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These volumes provide charts and background information summaries for MEG Categories 1-12 and 13-26. They address 586 organic compounds. In the context of deriving MEGs, the volumes: (1) offer perspective on the broad range of contaminants whose control is of vital interest to both industry and the public; (2) further develop and define indicators designating contaminants to be given priority consideration for immediate control and for subsequent research; (3) bring together existing and emerging data in a format efficient for use in environmental assessment; and (4) explore some basic methodologies which both provide the present goals, and suggest directions for refined methodologies. MEGs (multimedia environmental goals) are levels of significant contaminants or degradents (in ambient air, water, or land or in emissions of effluents conveyed to the ambient media) that are judged to be (1) appropriate for preventing certain negative effects in the surrounding populations or ecosystems, or (2) representative of the control limits achievable through technology. MEGs are predicted for more than 650 pollutants.

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ABSTRACT

Multimedia Environmental Goals (MEG's) are levels of significant contaminants or degradents (in ambient air, water, or land or in emissions of effluents conveyed to the ambient media) that are judged to be (1) appropriate for preventing certain negative effects in the surrounding populations or ecosystems, or (2) representative of the control limits achievable through technology. MEG's are projected for more than 650 pollutants. Volumes III and IV address 586 organic compounds.

In the context of deriving MEG's, these volumes attempt (1) to offer perspective on the broad range of contaminants whose control is of vital interest to both industry and the public; (2) to further develop and define indicators designating which contaminants must be given priority consideration for immediate control and for subsequent research; (3) to bring existing and emerging data together in a format efficient for use in environmental assessment; and (4) to explore some basic methodologies which provide the present goals, and which also suggest directions for refined methodologies.

CONTENTS

Abstract ii
Preferred Names and Synonyms for Organic Compounds Addressed by MEG's iv
Molecular Formula Index for Organic Compounds Addressed by MEG's xxviii
Appendix A MEG Charts and Background Information Summaries xxxv
  Category 13 Thiols, Sulfides, Disulfides A-483
  Category 14 Sulfonic Acids, Sulfoxides A-509
  Category 15 Benzene, Substituted Benzene Hydrocarbons A-519
  Category 16 Halogenated Aromatic Compounds A-561
  Category 17 Aromatic Nitro Compounds A-593
  Category 18 Phenols A-611
  Category 19 Halogenated Phenolic Compounds A-659
  Category 20 Nitrophenols A-673
  Category 21 Fused Polycyclic Hydrocarbons A-693
  Category 22 Fused Non-alternant Polycyclic Hydrocarbons A-775
  Category 23 Heterocyclic Nitrogen Compounds A-811
  Category 24 Heterocyclic Oxygen Compounds A-891
  Category 25 Heterocyclic S Compounds A-911
  Category 26 Organophosphorus Compounds A-931

PREFERRED NAMES AND SYNONYMS FOR ORGANIC COMPOUNDS ADDRESSED BY MEG'S

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
Acenaphthene	21A100	Acenaphthene
1-Acenaphthol	18C100	1-Acenaphthol
Acenaphthylene	21A120	Acenaphthylene
Acetaldehyde	07A040	Acetaldehyde
Acetamide	08C040	Acetamide
Acetic acid	08A040	Acetic acid
Acetic acid amide	08C040	Acetamide
Acetic aldehyde	07A040	Acetaldehyde
Acetone	07B020	Acetone
Acetone dichloride	02A344	2,2-Dichloropropane
Acetonitrile	09A020	Acetonitrile
Acetophenone	07B120	Acetophenone
Acetylbenzene	07B120	Acetophenone
Acetylene	01C020	Acetylene
Acetylene dichloride	02B040	1,2-Dichloroethene
Acetylene tetrachloride	02A300	1,1,2,2-tetrachloroethane
Acridan	23B100	Dihydroacridine
Acridine	23B080	Acridine
Acrolein	07A060	Acrolein
Acrolein dichloride	02B106	3,3-Dichloropropene
Acrylic aldehyde	07A060	Acrolein
Acrylon	09A040	Acrylonitrile
Acrylonitrile	09A040	Acrylonitrile
Active amyl alcohol	05A122	2-Methyl-1-butanol
Adipic acid	08A180	Adipic acid
Aerothene TT	02A280	Trichloroethane
Alkanes (C = 10, 11)	01A240	Alkanes (C = 10, 11)
Allylamine	10A110	3-Aminopropene
3-Amino propylene	10A110	3-Aminopropene
Amino-methane	10A020	Methylamine
2-Amino-1-propanol	10A121	2-Amino-1-propanol
3-Amino-1-propanol	10A122	3-Amino-1-propanol
4-Amino-1,2-dimethyl benzene	10C065	3,4-Xylidine
2-Amino-1,3-dimethyl benzene	10C064	2,6-Xylidine
2-Amino-1,4-dimethyl benzene	10C063	2,5-Xylidine
2-Amino-2-methylpropane	10A143	2-Amino-2-methylpropane
1-Amino-2-propanol	10A123	1-Amino-2-propanol
1-Amino-2,3-dimethyl benzene	10C061	2,3-Xylidine
1-Amino-2,4-dimethyl benzene	10C062	2,4-Xylidine
Di[-4-amino-3-chlorophenyl]methane	10C180	4,4'-Methylene bis(2-chloroaniline)
1-Amino-3,5-dimethyl benzene	10C066	3,5-Xylidine
2-Amino-4,6-dinitrophenol	20A080	2-Amino-4,6-dinitrophenol
4-Aminoaniline	10C100	1,4-Diaminobenzene
Aminoanisole	10C080	Anisidines
2-Aminoanisole	10C081	o-Anisidine
4-Aminoanisole	10C083	p-Anisidine
Aminobenzene	10C020	Aniline
4-Aminobiphenyl	10C120	4-Aminobiphenyl
1-Aminobutane	10A141	1-Aminobutane
2-Aminobutane	10A142	2-Aminobutane
Aminobutanes	10A140	Butylamines
Aminocaproic acid	08B100	6-Aminohexanoic acid
6-Aminocaproic acid	08B100	6-Aminohexanoic acid
Aminocyclohexane	10A160	Cyclohexylamine
Aminodimethylbenzenes	10C060	Dimethylanilines
1-Aminoethane	10A040	Ethlyamine
2-Aminoethanol	10A060	Ethanolamine
6-Aminohexanoic acid	08B100	6-Aminohexanoic acid
6-Aminohexanoic lactam	08C060	6-Hexanelactam
1-Aminonaphthalene	10C200	1-Aminonaphthalene
2-Aminonaphthalene	10C220	2-Aminonaphthalene
1-Aminopropane	10A100	1-Aminopropane
3-Aminopropene	10A110	3-Aminopropene
2-Aminopropylalcohol	10A121	2-Amino-1-propanol
2-Aminotoluene	10C041	2-Aminotoluene
3-Aminotoluene	10C042	3-Aminotoluene

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
4-Aminotoluene	10C043	4-Aminotoluene
Aminotoluenes	10C040	Aminotoluenes
n-Amyl acetate	08D141	n-Amyl acetate
sec-Amyl acetate	08D142	sec-Amyl acetate
Amyl acetates	08D140	Amyl acetates
Amyl acetic ether	08D141	n-Amyl acetate
Amyl alcohol	05A121	n-Pentanol
sec-Amyl alcohol	05B061	2-Pentanol
t-Amyl alcohol	05C040	t-Pentanol
Amyl alcohols	05A120	Pentanols, (primary)
Amyl alcohols	05B060	Pentanols, (secondary)
Amyl hydride	01A101	n-Pentane
a-n-Amylene	01B101	1-Pentene
cis-B-n-Amylene	01B102	cis-2-Pentene
trans-B-n-Amylene	01B103	trans-2-Pentene
Amylenes	01B100	Pentenes
Di-n-amylnitrosamine	12A100	N-Nitrosodipentylamine
Aniline	10C020	Aniline
o-Anisidine	10C081	o-Anisidine
m-Anisidine	10C082	m-Anisidine
p-Anisidine	10C083	p-Anisidine
Anisidines	10C080	Anisidines
Anthracene	21A140	Anthracene
2-Anthracenethiol	13A121	2-Anthracenethiol
9-Anthracenethiol	13A122	9-Anthracenethiol
Anthracenethiols	13A120	Anthracenethiols
Anthraquinone-disulfonic acids	14A040	Anthraquinone-disulfonic acids
9,10-Anthraquinone-1,5-disulfonic acid	14A041	9,10-Anthraquinone-1,5-disulfonic acid
9,10-Anthraquinone-1,6-disulfonic acid	14A042	9,10-Anthraquinone-1,6-disulfonic acid
9,10-Anthraquinone-1,7-disulfonic acid	14A043	9,10-Anthraquinone-1,7-disulfonic acid
9,10-Anthraquinone-1,8-disulfonic acid	14A044	9,10-Anthraquinone-1,8-disulfonic acid
Aroclors	16A220	Polychlorinated biphenyls (PCB's)
1-Aza-2,4-cyclopentadiene	23C020	Pyrrole
10-Azaanthracene	23B080	Acridine
Azabenzene	23A020	Pyridine
Azacyclopropane	10B020	Ethyleneimine
2-Azafluoranthene	23B300	Indeno(1,2,3-ij)isoquinoline
9-Azafluorene	23C080	Carbazole
1-Azaindene	23C040	Indole
9-Azaphenanthrene	23B120	Phenanthridine
Azimethylene	11A020	Diazomethane
Azine	23A020	Pyridine
Aziridine	10B020	Ethyleneimine
Azole	23C020	Pyrrole
B(a)P	21C100	Benzo(a)pyrene
B(b)F	22C080	Benzo(b)fluoranthene
B(j)F	22C040	Benzo(j)fluoranthene
BA	21B040	Benz(a)anthracene
Banana oil	08D143	Isoamyl acetate
Benz(a)acridine	23B120	Benz(a)acridine
Benz(a)acridine	23B180	Benz(a)acridine
Benz(a)anthracene	21B040	Benz(a)anthracene
Benz(a)anthrene-7(12H)one	07B160	5,6-Benzo-9-anthrone
Benz(a)phenanthrene	21B120	Chrysene
Benz(c)acridine	23B200	Benz(c)acridine
Benz(c)acridine	23B200	Benz(c)acridine
Benz(e)acephenantrylene	22C080	Benzo(b)fluoranthene
1,2-Benz-10-anthrone	07B160	5,6-Benzo-9-anthrone
2,3-Benz-4-azafluorene	23B280	2,3-Benz-4-azafluorene
1,2-Benzacridine	23B180	Benz(a)acridine
3,4-Benzacridine	23B200	Benz(c)acridine
Benzaldehyde	07A140	Benzaldehyde
2,3-Benzanthracene	21B020	Naphthacene
1,2-Benzanthracene	21B040	Benz(a)anthracene
1-Benzazine	23B021	Quinoline
1-Benzazole	23C040	Indole

6<

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
1,2-Benzcarbazole	23C120	Benzo(a)carbazole
Benzene	15A020	Benzene
Benzene carbinol	05A140	Benzyl alcohol
g-Benzene hexachloride	02A380	Hexachlorocyclohexane
Benzene methanol	05A140	Benzyl alcohol
Benzene-trans-hexachloride	02A380	Hexachlorocyclohexane
Benzenecarbinal	07A140	Benzaldehyde
Benzenecarboxylic acid	08A160	Benzoic acid
1,4-Benzenediamine	10C100	1,4-Diaminobenzene
1,2-Benzenedicarboxylic acid	08A200	Phthalic acid
o-Benzenediol	18B020	Catechol
m-Benzenediol	18B040	1,3-Dihydroxybenzene
1,4-Benzenediol	18B060	1,4-Dihydroxybenzene
Benzenesulfonic acid	14A020	Benzenesulfonic acid
Benzenetetrahydride	01B160	Cyclohexene
Benzenethiol	13A100	Benzenethiol
1,2,3-Benzenetriol	18B080	1,2,3-Trihydroxybenzene
8,9-Benzfluoranthene	22C020	Benzo(k)fluoranthene
7,8-Benzfluoranthene	22C040	Benzo(j)fluoranthene
Benzidine	10C140	Benzidine
4,5-Benzindane	22A040	Cyclopentanonaphthalene
2,3-Benzindene	22A020	Fluorene
Benzino form	02A240	Carbon Tetrachloride
Benzo(a)carbazole	23C120	Benzo(a)carbazole
11 H-Benzo(a)carbazole	23C120	Benzo(a)carbazole
Benzo(a)fluorene	22B060	1,2-Benzofluorene
11-HBenzo(a)fluorene	22B060	1,2-Benzofluorene
Benzo(a)pyrene	21C100	Benzo(a)pyrene
Benzo(b)anthracene	21B020	Naphthacene
Benzo(b)fluoranthene	22C080	Benzo(b)fluoranthene
Benzo(b)fluorene	22B020	2,3-Benzofluorene
11-HBenzo(b)fluorene	22B020	2,3-Benzofluorene
Benzo(b)naphtho(1,2-d)thiophene	25B082	Benzo(b)naphtho(1,2-d)thiophene
Benzo(b)naphtho(2,1-d)thiophene	25B083	Benzo(b)naphtho(2,1-d)thiophene
Benzo(b)naphtho(2,3-d)furan	24B060	Benzo(b)naphtho(2,3-d)furan
Benzo(b)naphtho(2,3-d)thiophene	25B081	Benzo(b)naphtho(2,3-d)thiophene
Benzo(b)phenanthrene	21B040	Benz(a)anthracene
Benzo(b)pyridine	23B021	Quinoline
Benzo(b)quinoline	23B080	Acridine
Benzo(b)thiophene	25B040	Benzo(b)thiophene
Benzo(b)triphenylene	21C060	Dibenz(a,c)anthracene
Benzo(c)phenanthrene	21B101	Benzo(c)phenanthrene
Benzo(c)phenanthrene and Alkyl derivatives	21B100	Benzo(c)phenanthrene and Alkyl derivatives
Benzo(c)pyridine	23B022	Isoquinoline
Benzo(c)quinoline	23B120	Phenanthridine
Benzo(def)phenanthrene	21B180	Pyrene
Benzo(e)pyrene	21C120	Benzo(e)pyrene
Benzo(f)quinoline	23B140	Benzo(f)quinoline
Benzo(g)chrysene	21C040	Benzo(g)chrysene
Benzo(ghi)perylene	21D080	Benzo(ghi)perylene
Benzo(h)quinoline	23B160	Benzo(h)quinoline
Benzo(j)fluoranthene	22C040	Benzo(j)fluoranthene
Benzo(j,k)fluorene	22B040	Fluoranthene
Benzo(k)fluoranthene	22C020	Benzo(k)fluoranthene
Benzo(k)xanthene	24B100	1,9-Benzoxanthene
Benzo(rst)pentaphene	21D040	Dibenzo(a,i)pyrene
5,6-Benzo-9-anthrone	07B160	5,6-Benzo-9-anthrone
11,12-Benzofluoranthene	22C020	Benzo(k)fluoranthene
10,11-Benzofluoranthene	22C040	Benzo(j)fluoranthene
2,3-Benzofluoranthene	22C080	Benzo(b)fluoranthene
2,3-Benzofluorene	22B020	2,3-Benzofluorene
1,2-Benzofluorene	22B060	1,2-Benzofluorene
Benzofuran	24A040	Benzofuran
Benzoic acid	08A160	Benzoic acid
Benzoic acid phenyl ester	08D180	Phenyl benzoate
Benzoic aldehyde	07A140	Benzaldehyde

7<

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
Benzol	15A020	Benzene
1,2-Benzonaphthacene	21C020	1,2-Benzonaphthacene
Benzonaphthathiophenes	25B080	Benzonaphthathiophenes
Benzonitrile	09B020	Benzonitrile
1,12-Benzoperylene	21D080	Benzo(ghi)perylene
2,3-Benzophenanthrene	21B040	Benz(a)anthracene
1,2-Benzophenanthrene	21B120	Chrysene
9,10-Benzophenanthrene	21B160	Triphenylene
4,5-Benzopyrene	21C120	Benzo(e)pyrene
2,3-Benzopyrrole	23C040	Indole
3,4-Benzoquinoline	23B120	Phenanthridine
5,6-Benzoquinoline	23B140	Benzo(f)quinoline
7,8-Benzoquinoline	23B160	Benzo(h)quinoline
Benzosulfonazole	23D020	Benzothiazole
Benzothiazole	23D020	Benzothiazole
Benzothiofuran	25B040	Benzo(b)thiophene
2,3-Benzothiophene	25B040	Benzo(b)thiophene
1,9-Benzoxanthene	24B100	1,9-Benzoxanthene
Benzoyl alcohol	05A140	Benzyl alcohol
1,2-Benzpyrene	21C100	Benzo(a)pyrene
3,4-Benzpyrene	21C100	Benzo(a)pyrene
1,2-Benzpyrene	21C120	Benzo(e)pyrene
Benzyl alcohol	05A140	Benzyl alcohol
Benzyl carbinol	05A160	Phenethyl alcohol
Benzyl chloride	16B020	a-Chlorotoluene
Betaprone	08B060	b-Propiolactone
Bibenzene	15A160	Biphenyl
Bicyclopentadiene	01B220	Dicyclopentadiene
Bimethyl	01A040	Ethane
Biphenyl	15A160	Biphenyl
4-Biphenylamine	10C120	4-Aminobiphenyl
2,2'-Biphenyldiol	18A120	2,2'-Dihydroxydiphenyl
Biphenylols	18A100	Phenylphenols
Biscyclopentadiene	01B220	Dicyclopentadiene
Bisoflex	08D260	Di-2-ethylhexyl adipate
2,2'-Bithienyl	25B020	2,2'-Bithiophene
2,2'-Bithiophene	25B020	2,2'-Bithiophene
Bivinyl	01B082	1,3-Butadiene
2-Bornanone	07B100	Camphor
Borneo camphor	05B120	Borneol
Borneol	05B120	Borneol
Bornyl alcohol	05B120	Borneol
BPL	08B060	b-Propiolactone
b-Brazan	24B060	Benzo(b)naphtho(2,3-d)furan
1-Bromo-2-chlorobenzene	16A081	1-Bromo-2-chlorobenzene
2-Bromo-2-methylpropane	02A363	2-Bromoisobutane
1-Bromo-3-chlorobenzene	16A082	1-Bromo-3-chlorobenzene
1-Bromo-4-chlorobenzene	16A083	1-Bromo-4-chlorobenzene
Bromobenzene	16A040	Bromobenzene
1-Bromobutane	02A361	1-Bromobutane
2-Bromobutane	02A362	2-Bromobutane
Bromobutanes	02A360	Bromobutanes
Bromochlorobenzenes	16A080	Bromochlorobenzenes
Bromodichloromethane	02A120	Bromodichloromethane
Bromoform	02A160	Bromoform
2-Bromoisobutane	02A363	2-Bromoisobutane
4-Bromophenyl phenyl ether	04A200	4-Bromophenyl phenyl ether
Buta-1,3-diene	01B082	1,3-Butadiene
1,2-Butadiene	01B081	1,2-Butadiene
1,3-Butadiene	01B082	1,3-Butadiene
Butadienes	01B080	Butadienes
Butanal	07A100	Butyraldehyde
n-Butane	01A081	n-Butane
Butanecarboxylic acid	08A080	Valeric acid
1,4-Butanedicarboxylic acid	08A180	Adipic acid
Butanes	01A080	Butanes

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
n-Butanethiol	13A080	n-Butanethiol
1-Butanethiol	13A080	n-Butanethiol
Butanitrile	09A080	Butyronitrile
n-Butanol	05A080	n-Butanol
1-Butanol	05A080	n-Butanol
2-Butanol	05B040	2-Butanol
t-Butanol	05C020	t-Butyl alcohol
Butanone	07B060	Butanone
2-Butanone	07B060	Butanone
1-Butene	01B061	1-Butene
cis-2-Butene	01B062	cis-2-Butene
trans-2-Butene	01B063	trans-2-Butene
cis-Butenedioic acid	08A060	Maleic acid
Butric aldehyde	07A100	Butyraldehyde
Butter or methyl yellow	11A040	p-Dimemthylaminoazobenzene
n-Butyl acetate	08D121	n-Butyl acetate
sec-Butyl acetate	08D122	sec-Butyl acetate
Butyl acetates	08D120	Butyl acetates
Butyl adipate	08D220	Dibutyl adipate
Di-N-butyl adipate	08D220	Dibutyl adipate
Butyl alcohol	05A080	n-Butanol
sec-Butyl alcohol	05B040	2-Butanol
t-Butyl alcohol	05C020	t-Butyl alcohol
n-Butyl aldehyde	07A100	Butyraldehyde
n-Butyl benzene	15A141	n-Butyl benzene
sec-Butyl benzene	15A142	sec-Butyl benzene
sec-Butyl benzene	15A142	sec-Butyl benzene
tert-Butyl benzene	15A143	tert-Butyl benzene
tert-Butyl benzene	15A143	tert-Butyl benzene
Butyl benzenes	15A140	Butyl benzenes
Butyl benzenes	15A140	Butyl benzenes
Butyl benzyl phthalate	08D320	Butyl benzyl phthalate
Butyl ethanoate	08D121	n-Butyl acetate
n-Butyl mercaptan	13A080	n-Butanethiol
Di-n-butyl phthalate	08D283	Di-n-butyl Phthalate
n-Butylamine	10A141	1-Aminobutane
Butylamines	10A140	Butylamines
n-Butylbromide	02A361	1-Bromobutane
sec-Butylbromide	02A362	2-Bromobutane
tert-Butylbromide	02A363	2-Bromoisobutane
a-Butylene	01B061	1-Butene
cis-B-Butylene	01B062	cis-2-Butene
trans-B-Butylene	01B063	trans-2-Butene
Butylenes	01B060	Butylenes
Butylethylene	01B141	1-Hexene
n-Butylthioalcohol	13A080	n-Butanethiol
1-Butyne	01C061	1-Butyne
2-Butyne	01C062	2-Butyne
Butynes	01C060	Butynes
Butyraldehyde	07A100	Butyraldehyde
g-Butyrolactone	08B080	g-Butyrolactone
4-Butyrolactone	08B080	g-Butyrolactone
Butyronitrile	09A080	Butyronitrile
C-56	02B140	Hexachlorocyclopentadiene
a,b-Camphol	05B140	Isoborneol
d-2-Camphonone	07B100	Camphor
2-Camphonone	07B100	Camphor
Camphor	07B100	Camphor
Capric acid	08A103	Capric acid
Caproic acid	08A101	Caproic acid
e-Caprolactam	08C060	6-Hexanelactam
Caprylic acid	08A102	Caprylic acid
Carbazine	23B100	Dihydroacridine
Carbazole	23C080	Carbazole
Carbinol	05A020	Methanol
Carbolic acid	18A020	Phenol

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
Carbon bichloride	02B080	Tetrachloroethene
Carbon dichloride	02B080	Tetrachloroethene
Carbon hexachloride	02A320	Hexachloroethane
Carbon tetrachloride	02A240	Carbon tetrachloride
Carvol	07B181	Carvone (d or l)
Carvone (d or l)	07B181	Carvone (d or l)
Carvones	07B180	Carvones
Catechol	18B020	Catechol
Cetylic acid	08A122	Palmitic acid
Chinoline	23B021	Quinoline
Chlorinated cresols	19B020	Chlorinated cresols
Chlorinated-m-cresol	19B022	Chlorinated m-cresol
Chlorinated-o-cresol	19B021	Chlorinated o-cresol
Chlorinated-p-cresol	19B023	Chlorinated p-cresol
bis-(2-Chloro-1-methylethyl)ether	04B100	2,2'-Dichlorodiisopropyl ether
2-Chloro-1,2-epoxypropane	04A040	2-Chloro-1,2-epoxypropane
1-Chloro-1,2-oxetane	04A060	1-Chloro-1,3-epoxypropane
1-Chloro-1,3-epoxypropane	04A060	1-Chloro-1,3-epoxypropane
4-Chloro-2-hydroxy benzophenone	07C04A	4-Chloro-2-hydroxy benzophenone
4-Chloro-2'-hydroxy benzophenone	07C04B	4-Chloro-2'-hydroxy benzophenone
5-Chloro-2-hydroxy benzophenone	07C04E	5-Chloro-2-hydroxy benzophenone
2-Chloro-2'-hydroxy benzophenone	07C041	2-Chloro-2'-hydroxy benzophenone
3-Chloro-2'-hydroxy benzophenone	07C045	3-Chloro-2'-hydroxy benzophenone
3-Chloro-2-hydroxy benzophenone	07C046	3-Chloro-2-hydroxy benzophenone
1-Chloro-2-nitrobenzene	17B040	1-Chloro-2-nitrobenzene
1-Chloro-2,3-epoxypropane	04A050	Epichlorhydrin
4-Chloro-3'-hydroxy benzophenone	07C04C	4-Chloro-3'-hydroxy benzophenons
2-Chloro-3'-hydroxy benzophenone	07C042	2-Chloro-3'-hydroxy benzophenonen
3-Chloro-3'-hydroxy benzophenone	07C047	3-Chloro-3'-hydroxy benzophenone
4-Chloro-4'-hydroxy benzophenone	07C04D	4-Chloro-4'-hydroxy benzophenone
2-Chloro-4'-hydroxy benzophenone	07C043	2-Chloro-4'-hydroxy benzophenone
3-Chloro-4'-hydroxy benzophenone	07C048	3-Chloro-4'-hydroxy benzophenone
3-Chloro-4-hydroxy benzophenone	07C049	3-Chloro-4-hydroxy benzophenone
1-Chloro-4-nitrobenzene	17B060	1-Chloro-4-nitrobenzene
2-Chloro-5-hydroxy benzophenone	07C044	2-Chloro-5-hydroxy benzophenone
a-Chloroallychloride	02B103	cis-1,3-Dichloropropene
Chlorobenzene	16A020	Chlorobenzene
a-Chlorobutyl ethyl ether	04A160	a-Chlorobutyl ethyl ether
Chlorodibromomethane	02A140	Dibromochloromethane
2-Chlorodiethyl ether	04A120	2-Chloroethyl ethyl ether
Chloroethane	02A250	Ethyl chloride
Chloroethene	02B020	Vinyl chloride
Chloroethyl	02A250	Ethyl chloride
2-Chloroethyl ethyl ether	04A120	2-Chloroethyl ethyl ether
2-Chloroethyl vinyl ether	04A140	2-Chloroethyl vinyl ether
bis-(2-Chloroethyl)ether	04B080	2,2'-Dichlorodiethyl ether
Chloroethylene	02B020	Vinyl chloride
2-Chloroethylmethyl ether	04A080	2-Chloroethylmethyl ether
Chloroform	02A100	Chloroform
Chlorohydroxy benzophenones	07C040	Chlorohydroxy benzophenones
Chlorohydroxytoluenes	19B020	Chlorinated cresols
bis(a-Chloroisopropyl)ether	04B100	2,2'-Dichlorodiisopropyl ether
Chloromethane	02A040	Methyl chloride
Chloromethyl ethyl ether	04A100	Chloromethyl ethyl ether
Chloromethyl methyl ether	04A020	Chloromethyl methyl ether
(Chloromethyl)benzene	16B020	a-Chlorotoluene
1,2-bis(Chloromethyl)benzene	16B041	1,2-bis (Chloromethyl) benzene
1,3-bis(Chloromethyl)benzene	16B042	1,3-bis (Chloromethyl) benzene
1,4-bis(Chloromethyl)benzene	16B043	1,4-bis (Chloromethyl) benzene
bis (Chloromethyl)benzenes	16B040	bis (Chloromethyl) benzenes
bis(Chloromethyl)ether	04B020	1,1'-Dichloromethyl ether
Chloromethyloxirane	04A050	Epichlorhydrin
1-Chloronaphthalene	16A201	1-Chloronaphthalene
a-Chloronaphthalene	16A201	1-Chloronaphthalene
2-Chloronaphthalene	16A202	2-Chloronaphthalene
b-Chloronaphthalene	16A202	2-Chloronaphthalene

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
Chloronaphthalenes	16A200	Chloronaphthalenes
o-Chloronitrobenzene	17B040	1-Chloro-2-nitrobenzene
p-Chloronitrobenzene	17B060	1-Chloro-4-nitrobenzene
1-Chlorooctane	02A400	1-Chlorooctane
Chlorophen	19A060	Pentachlorophenol
2-Chlorophenol	19A020	2-Chlorophenol
o-Chlorophenol	19A020	2-Chlorophenol
4-Chlorophenyl phenyl ether	04A180	4-Chlorophenyl phenyl ether
g-Chloropropylene oxide	04A050	Epichlorhydrin
2-Chloropyridine	23A101	2-Chloropyridine
3-Chloropyridine	23A102	3-Chloropyridine
4-Chloropyridine	23A103	4-Chloropyridine
Chloropyridines	23A100	Chloropyridines
Chlorothene	02A280	Trichloroethane
2-Chlorotoluene	16A180	2-Chlorotoluene
o-Chlorotoluene	16A180	2-Chlorotoluene
a-Chlorotoluene	16B020	a-Chlorotoluene
Chlorten	02A280	Trichloroethane
Chrysene	21B120	Chrysene
a-Chrysidine	23B200	Benz(c)acridine
a-Chrysidine	23B200	Benz(c)acridine
Chrysofluorene	22B060	1,2-Benzofluorene
Chrysogen	21B020	Napthacene
CMME	04A020	Chloromethyl methyl ether
2,4,6-Collidine	23A122	2,4,6-Collidine
Collidines	23A120	Collidines
Coronene	21D100	Coronene
Coumarone	24A040	Benzofuran
m-Cresol	18A041	m-Cresol
o-Cresol	18A042	o-Cresol
p-Cresol	18A043	p-Cresol
Cresols	18A040	Cresols
Cresylic acid	18A040	Cresols
Crotonylene	01C062	2-Butyne
Cumarone	24A040	Benzofuran
Cumeme	15A120	Isopropyl benzene
Cyanobenzene	09B020	Benzonitrile
1-Cyanoethane	09A060	1-Cyanoethane
Cyanoethylene	09A040	Acrylonitrile
1-Cyanonaphthalene	09B041	a-Naphthonitrile
2-Cyanonaphthalene	09B042	b-Naphthonitrile
Cyanonaphthalenes	09B040	Naphthonitriles
Cyanopropane	09A080	Butyronitrile
1,3-Cyclohexadiene	01B181	1,3-Cyclohexadiene
1,4-Cyclohexadiene	01B182	1,4-Cyclohexadiene
Cyclohexadienes	01B180	Cyclohexadienes
Cyclohexane	01A160	Cyclohexane
Cyclohexene	01B160	Cyclohexene
Cyclohexylamine	10A160	Cyclohexylamine
Cyclopenta(def)phenanthrene	22B080	Cyclopenta(def)phenanthrene
4H-Cyclopenta(def)phenanthrene	22B080	Cyclopenta(def)phenanthrene
Cyclopentadiene	01B120	Cyclopentadiene
1,3-Cyclopentadiene	01B120	Cyclopentadiene
1,3-Cyclopentadiene dimer	01B220	Dicyclopentadiene
Cyclopentane	01A120	Cyclopentane
1,2-Cyclopentanonaphthalene	22A040	Cyclopentanonaphthalene
Cyclopentanonaphthalene	22A040	Cyclopentanonaphthalene
Cyclotetramethylene oxide	03A060	Tetrahydrofuran
b-Cytisolidine	23B065	6,8-Dimethylquinoline
DB(a,h)A	21C080	Dibenz(a,h)anthracene
DB(a,h)P	21D020	Dibenzo(a,h)pyrene
n-Decane	01A241	n-Decane
n-Decanoic acid	08A103	Capric acid
n-Decoic acid	08A103	Capric acid
Decylhydride	01A241	n-Decane
2,6-Di-sec-butyl phenol	18A182	2,6-Di-sec-butyl phenol

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
1,4-Di-tert-butyl benzene	15B106	1,4-Di-tert-butyl benzene
Di-2-ethylbutyl adipate	08D240	Di-2-ethylbutyl adipate
Di-2-ethylhexyl adipate	08D260	Di-2-ethylhexyl adipate
Di-2-ethylhexyl phthalate	08D300	Di-2-ethylhexyl phthalate
Dialkyl benzenes (MW:134-191)	15B100	Dialkyl benzenes (MW:134-191)
4,4'-Diamino-3,3'-dichlorobiphenyl	10C160	3,3'-Dichlorobenzidine
1,4-Diaminobenzene	10C100	1,4-Diaminobenzene
p-Diaminobenzene	10C100	1,4-Diaminobenzene
4,4'-Diaminodiphenyl	10C140	Benzidine
1,2-Diaminoethane	10A080	1,2-Diaminoethane
Diazirine	11A020	Diazomethane
Diazomethane	11A020	Diazomethane
Dibenz(a,c)anthracene	21C060	Dibenz(a,c)anthracene
Dibenz(a,h)acridine	23B240	Dibenz(a,h)acridine
Dibenz(a,h)anthracene	21C080	Dibenz(a,h)anthracene
Dibenz(a,j)acridine	23B220	Dibenz(a,j)acridine
Dibenz(a,j)anthracene	21C020	1,2-Benzonaphthacene
Dibenz(b,d)pyrrole	23C080	Carbazole
Dibenz(c,h)acridine	23B260	Dibenz(c,h)acridine
Dibenz(de,kl)anthracene	21C140	Perylene
1,2:7,8-Dibenzacridine	23B220	Dibenz(a,j)acridine
1,2:5,6-Dibenzacridine	23B240	Dibenz(a,h)acridine
3,4:5,6-Dibenzacridine	23B260	Dibenz(c,h)acridine
1,2:6,7-Dibenzanthracene	21C020	1,2-Benzonaphthacene
1,2:3,4-Dibenzanthracene	21C060	Dibenz(a,c)anthracene
1,2:5,6-Dibenzanthracene	21C080	Dibenz(a,h)anthracene
1,2:3,4-Dibenznaphthalene	21B160	Triphenylene
Dibenzo(a,g)carbazole	23C180	Dibenzo(a,g)carbazole
7H-Dibenzo(a,g)carbazole	23C180	Dibenzo(a,g)carbazole
13H-Dibenzo(a,g)fluorene	22C060	1,2:5,6-Dibenzo fluorene
Dibenzo(a,h)pyrene	21D020	Dibenzo(a,h)pyrene
Dibenzo(a,i)carbazole	23C140	Dibenzo(a,i)carbazole
7H-Dibenzo(a,i)carbazole	23C140	Dibenzo(a,i)carbazole
Dibenzo(a,i)phenanthrene	21C160	Picene
Dibenzo(a,i)pyrene	21D040	Dibenzo(a,i)pyrene
Dibenzo(a,l)pyrene	21D060	Dibenzo(a,l)pyrene
Dibenzo(b,def)chrysene	21D020	Dibenzo(a,h)pyrene
Dibenzo(b,e)pyridine	23B080	Acridine
Dibenzo(c,g)carbazole	23C160	Dibenzo(c,g)carbazole
7H-Dibenzo(c,g)carbazole	23C160	Dibenzo(c,g)carbazole
Dibenzo(def,p)chrysene	21D060	Dibenzo(a,l)pyrene
1,2:7,8-Dibenzocarbazole	23C140	Dibenzo(a,i)carbazole
3,4:5,6-Dibenzocarbazole	23C160	Dibenzo(c,g)carbazole
1,2:5,6-Dibenzocarbazole	23C180	Dibenzo(a,g)carbazole
1,2:5,6-Dibenzofluorene	22C060	1,2:5,6-Dibenzofluorene
Dibenzofuran	24B020	Dibenzofuran
1,2:3,4-Dibenzophenanthrene	21C040	Benzo(g)chrysene
1,2:9,10-Dibenzopyrene	21D060	Dibenzo(a,l)pyrene
Dibenzothiophene	25B060	Dibenzothiophene
1,2:7,8-Dibenzphenanthrene	21C160	Picene
1,2:6,7-Dibenzpyrene	21D020	Dibenzo(a,h)pyrene
3,4:8,9-Dibenzpyrene	21D020	Dibenzo(a,h)pyrene
2,3:6,7-Dibenzpyrene	21D040	Dibenzo(a,i)pyrene
4,5:8,9-Dibenzpyrene	21D040	Dibenzo(a,i)pyrene
1,2:3,4-Dibenzpyrene	21D060	Dibenzo(a,l)pyrene
2,3:4,5-Dibenzpyrene	21D060	Dibenzo(a,l)pyrene
1,2-Dibromobenzene	16A061	1,2-Dibromobenzene
1,3-Dibromobenzene	16A062	1,3-Dibromobenzene
1,4-Dibromobenzene	16A063	1,4-Dibromobenzene
Dibromobenzenes	16A060	Dibromobenzenes
Dibromochloromethane	02A140	Dibromochloromethane
Dibromodichloromethane	02A180	Dibromodichloromethane
Dibutyl adipate	08D220	Dibutyl adipate
1,1-Dichloro-2,2-difluoroethene	02B090	1,1-Dichloro-2,2-difluoroethylene
1,1-Dichloro-2,2-difluoroethylene	02B090	1,1-Dichloro-2,2-difluoroethylene
3,3'-Dichloro-4,4'-biphenyldiamine	10C160	3,3'-Dichlorobenzidine

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
3,3'-Dichloro-4,4'-diaminobiphenyl	10C160	3,3'-Dichlorobenzidine
3,3'Dichloro-4,4'-diaminodiphenyl methane	10C180	4,4'-Methylene bis(2-chloroaniline)
1,2-Dichlorobenzene	16A100	1,2-Dichlorobenzene
o-Dichlorobenzene	16A100	1,2-Dichlorobenzene
1,3-Dichlorobenzene	16A120	1,3-Dichlorobenzene
m-Dichlorobenzene	16A120	1,3-Dichlorobenzene
1,4-Dichlorobenzene	16A140	1,4-Dichlorobenzene
p-Dichlorobenzene	16A140	1,4-Dichlorobenzene
3,3'-Dichlorobenzidine	10C160	3,3'-Dichlorobenzidine
o,o'-Dichlorobenzidine	10C160	3,3'-Dichlorobenzidine
Dichlorobromomethane	02A120	Bromodichloromethane
1,1'-Dichlorodiethyl ether	04B040	1,1'-Dichlorodiethyl ether
2,2'-Dichlorodiethyl ether	04B080	2,2'-Dichlorodiethyl ether
Dichlorodifluoromethane	02A200	Dichlorodifluoromethane
1,2-Dichlorodiisobutyl ether	04B120	1,2-Dichlorodiisobutyl ether
2,2'-Dichlorodiisopropyl ether	04B100	2,2'-Dichlorodiisopropyl ether
1,2-Dichloroethane	02A260	1,2-Dichloroethane
1,2-Dichloroethene	02B040	1,2-Dichloroethene
cis-1,2-Dichloroethene	02B041	cis-1,2-Dichloroethene
trans-1,2-Dichloroethene	02B042	trans-1,2-Dichloroethene
1,1-Dichloroethene	02B060	1,1-Dichloroethene
1,2-Dichloroethyl ethyl ether	04B060	1,2-Dichloroethyl ethyl ether
Dichloroethylene	02B040	1,2-Dichloroethene
1,1-Dichloroethylene	02B060	1,1-Dichloroethene
Dichloromethane	02A080	Methylene chloride
1,1'-Dichloromethyl ether	04B020	1,1'-Dichloromethyl ether
2,4-Dichlorophenol	19A040	2,4-Dichlorophenol
1,1-Dichloropropane	02A341	1,1-Dichloropropane
1,2-Dichloropropane	02A342	1,2-Dichloropropane
1,3-Dichloropropane	02A343	1,3-Dichloropropane
2,2-Dichloropropane	02A344	2,2-Dichloropropane
Dichloropropanes	02A340	Dichloropropanes
1,1-Dichloropropene	02B101	1,1-Dichloropropene
trans-1,2-Dichloropropene	02B102	trans-1,2-Dichloropropene
cis-1,3-Dichloropropene	02B103	cis-1,3-Dichloropropene
trans-1,3-Dichloropropene	02B104	trans-1,3-Dichloropropene
2,3-Dichloropropene	02B105	2,3-Dichloropropene
3,3-Dichloropropene	02B106	3,3-Dichloropropene
Dichloropropenes	02B100	Dichloropropenes
1,2-Dichloropropylene	02B102	trans-1,2-Dichloropropene
a,g-Dichloropropylene	02B103	cis-1,3-Dichloropropene
1,3-Dichloropropylene	02B103	cis-1,3-Dichloropropene
1,3-Dicyano-1-hydroxybutane	09A100	1,3-Dicyano-1-hydroxybutane
Dicyclopentadiene	01B220	Dicyclopentadiene
Diethamine	10B080	Diethylamine
Diethyl adipate	08D200	Diethyl adipate
o-Diethyl benzene	15B101	o-Diethyl benzene
m-Diethyl benzene	15B102	m-Diethyl benzene
p-Diethyl benzene	15B103	p-Diethyl benzene
Diethyl carbinol	05B062	3-Pentanol
Diethyl hexyl phthalate	08D300	Di-2-ethylhexyl phthalate
Diethyl phthalate	08D282	Diethyl phthalate
Diethyl sulfide	13B040	Diethyl sulfide
Diethylamine	10B080	Diethylamine
1,4-Diethylene dioxide	03B020	1,4-Dioxane
Diethylene imidoxide	10B100	Morpholine
Diethylene oximide	10B100	Morpholine
Diethyleneimide oxide	10B100	Morpholine
Diethylnitrosoamine	12A040	N-Nitrosodiethylamine
1,1-Difluoro-2,2-dichloroethylene	02B090	1,1-Dichloro-2,2-difluoroethylene
Difluorodichloromethane	02A200	Dichlorodifluoromethane
Dihexyl	01A260	n-Dodecane
Dihydro-(d or l)carvone	07B182	Dihydro-(d or l) carvone
Dihydro-2(3H)-furanone	08B080	g-Butyrolactone
1,2-Dihydro-3-methylbenz(j)aceanthrylene	21B080	3-Methylcholanthrene
1,2-Dihydroacenaphthylene	21A100	Acenaphthene

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
Dihydroacridine	23B100	Dihydroacridine
1,4-Dihydrobenzene	01B182	1,4-Cyclohexadiene
1,2-Dihydrobenzene	01B181	1,3-Cyclohexadiene
2,3-Dihydroindene	15B020	Indan
1,2-Dihydronaphthalene	15B141	1,2-Dihydronaphthalene
1,4-Dihydronaphthalene	15B142	1,4-Dihydronaphthalene
Dihydronaphthalenes	15B140	Dihydronaphthalenes
o-Dihydroxybenzene	18B020	Catechol
1,2-Dihydroxybenzene	18B020	Catechol
1,3-Dihydroxybenzene	18B040	1,3-Dihydroxybenzene
m-Dihydroxybenzene	18B040	1,3-Dihydroxybenzene
1,4-Dihydroxybenzene	18B060	1,4-Dihydroxybenzene
p-Dihydroxybenzene	18B060	1,4-Dihydroxybenzene
2,2'-Dihydroxydiphenyl	18A120	2,2'-Dihydroxydiphenyl
1,2-Dihydroxyethane	06A020	Ethylene glycol
1,2-Dihydroxypropane	06A040	Propylene glycol
Diisobutyl carbinol	05B080	2,6-Dimethyl-4-heptanol
o-Diisopropyl benzene	15B104	o-Diisopropyl benzene
m-Diisopropyl benzene	15B105	m-Diisopropyl benzene
Diisopropyl ether	03A020	Isopropyl ether
Dimazine	11B040	N,N-Dimethylhydrazine
3,4-diMe-thiophene	25A064	3,4-Dimethylthiophene
Dimethyl	01A040	Ethane
2,3-Dimethyl aniline	10C061	2,3-Xylidine
2,4-Dimethyl aniline	10C062	2,4-Xylidine
2,5-Dimethyl aniline	10C063	2,5-Xylidine
2,6-Dimethyl aniline	10C064	2,6-Xylidine
3,4-Dimethyl aniline	10C065	3,4-Xylidine
3,5-Dimethyl aniline	10C066	3,5-Xylidine
Dimethyl chloroether	04A020	Chloromethyl methyl ether
Dimethyl disulfide	13B080	Methyldisulfide
Dimethyl ethyl carbinol	05C040	t-Pentanol
2,6-Dimethyl heptan-4-ol	05B080	2,6-Dimethyl-4-heptanol
1,4-Dimethyl naphthalene	21A081	1,4-Dimethyl naphthalene
2,3-Dimethyl naphthalene	21A082	2,3-Dimethyl naphthalene
2,6-Dimethyl naphthalene	21A083	2,6-Dimethyl napthalene
Dimethyl naphthalenes	21A080	Dimethyl naphthalenes
Dimethyl phthalate	08D281	Dimethyl phthalate
3,4-Dimethyl pyrene	21B221	3,4-Dimethyl pyrene
4,5-Dimethyl pyrene	21B222	4,5-Dimethyl pyrene
Dimethyl pyrenes	21B220	Dimethyl pyrenes
Dimethyl sulfide	13B020	Dimethyl sulfide
Dimethyl sulfoxide	14B020	Dimethyl sulfoxide
2,4-Dimethyl-1-hydroxy benzene	18A142	2,4-Xylenol
2,2-Dimethyl-1-propanol	05A123	2,2-Dimethyl-1-propanol
9,10-Dimethyl-1,2-benzanthracene	21B060	7,12-Dimethylbenz(a)anthracene
1,4-Dimethyl-2-hydroxy benzene	18A143	2,5-Xylenol
1,3-Dimethyl-2-hydroxy benzene	18A144	2,6-Xylenol
1,2-Dimethyl-3-hydroxy benzene	18A141	2,3-Xylenol
N,N-Dimethyl-4-(phenylazo)benzenamine	11A040	p-Dimethylaminoazobenzene
2,6-Dimethyl-4-heptanol	05B080	2,6-Dimethyl-4-heptanol
2,6-Dimethyl-4-heptyl phenol	18A183	2,6-Dimethyl-4-heptyl phenol
1,2-Dimethyl-4-hydroxy benzene	18A146	3,4-Xylenol
1,3-Dimethyl-5-hydroxy benzene	18A145	3,5-Xylenol
Dimethylacetylene	01C062	2-Butyne
Dimethylamine	10B040	Dimethylamine
p-Dimethylaminoazobenzene	11A040	p-Dimethylaminoazobenzene
4-Dimethylaminoazobenzene	11A040	p-Dimethylaminoazobenzene
N,N-Dimethylaniline	10D020	N,N-Dimethylaniline
Dimethylanilines	10C060	Dimethylanilines
2,7-Dimethylanthracene	21A160	2,7-Dimethylanthracene
7,12-Dimethylbenz(a)anthracene	21B060	7,12-Dimethylbenz(a)anthracene
Dimethylbenzene	15B080	Xylenes
Dimethylenediamine	10A080	1,2-Diaminoethane
(1,1-Dimethylethyl)benzene	15A143	tert-Butyl benzene
(1,1-Dimethylethyl)benzene	15A143	tert-Butyl benzene

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
Dimethylethylene	01B062	cis-2-Butene
N,N-Dimethylhydrazine	11B040	N,N-Dimethylhydrazine
1,1-Dimethylhydrazine	11B040	N,N-Dimethylhydrazine
N,N'-Dimethylhydrazine	11B060	N,N'-Dimethylhydrazine
1,2-Dimethylhydrazine	11B060	N,N'-Dimethylhydrazine
Dimethylhydrazine	11B060	N,N'-Dimethylhydrazine
Dimethylhydroxybenzenes	18A140	Xylenols
1,3-Dimethylisoquinoline	23B066	1,3-Dimethylisoquinoline
1,5-Dimethylisquinoline	23B067	1,5-Dimethylisoquinoline
Dimethylketone	07B020	Acetone
Dimethylmethane	01A060	Propane
a-Dimethylnapthalene	21A081	1,4-Dimethyl naphthalene
Dimethylnitrosoamine	12A020	N-Nitrosodimethylamine
2,3-Dimethylphenol	18A141	2,3-Xylenol
2,4-Dimethylphenol	18A142	2,4-Xylenol
2,5-Dimethylphenol	18A143	2,5-Xylenol
2,6-Dimethylphenol	18A144	2,6-Xylenol
3,5-Dimethylphenol	18A145	3,5-Xylenol
3,4-Dimethylphenol	18A146	3,4-Xylenol
Dimethylphenols	18A140	Xylenols
Dimethylphenylamine	10D020	N,N-Dimethylaniline
2,2-Dimethylpropane	01A103	Neopentane
2,3-Dimethylpyridine	23A141	2,3-Dimethylpyridine
2,4-Dimethylpyridine	23A142	2,4-Dimethylpyridine
2,5-Dimethylpyridine	23A143	2,5-Dimethylpyridine
2,6-Dimethylpyridine	23A144	2,6-Dimethylpyridine
3,4-Dimethylpyridine	23A145	3,4-Dimethylpyridine
2,3-Dimethylquinoline	23B061	2,3-Dimethylquinoline
2,6-Dimethylquinoline	23B062	2,6-Dimethylquinoline
2,8-Dimethylquinoline	23B063	2,8-Dimethylquinoline
3,4-Dimethylquinoline	23B064	3,4-Dimethylquinoline
6,8-Dimethylquinoline	23B065	6,8-Dimethylquinoline
Dimethylquinolines and dimethylisoquinolines	23B060	Dimethyquinolines and dimethylisoquinolines
2,3-Dimethylthiophene	25A061	2,3-Dimethylthiophene
2,4-Dimethylthiophene	25A062	2,4-Dimethylthiophene
2,5-Dimethylthiophene	25A063	2,5-Dimethylthiophene
3,4-Dimethylthiophene	25A064	3,4-Dimethylthiophene
Dimethylthiophenes	25A060	Dimethylthiophenes
peri-Dinaphthalene	21C140	Perylene
4,6-Dinitro-o-cresol	20B020	4,6-Dinitro-o-cresol
2,4-Dinitro-o-cresol	20B020	4,6-Dintro-o-cresol
3,5-Dinitro-p-cresol	20B041	3,5-Dinitro-p-cresol
2,6-Dinitro-p-cresol	20B042	2,6-Dinitro-p-cresol
Dinitro-p-cresols	20B040	Dinitro-p-cresols
3,5-Dinitro-2-hydroxy toluene	20B020	4,6-Dinitro-o-cresol
Dinitroaminophenol	20A080	2-Amino-4,6-dinitrophenol
Dinitrohydroxybenzenes	20A100	Dinitrophenols
2,4-Dinitrophenol	20A101	2,4-Dinitrophenol
2,5-Dinitrophenol	20A102	2,5-Dinitrophenol
2,6-Dinitrophenol	20A103	2,6-Dinitrophenol
Dinitrophenols	20A100	Dinitrophenols
2,6-Dinitrotoluene	17A081	2,6-Dinitrotoluene
3,4-Dinitrotoluene	17A082	3,4-Dinitrotoluene
2,3-Dinitrotoluene	17A083	2,3-Dinitrotoluene
2,4-Dinitrotoluene	17A084	2,4-Dinitrotoluene
2,5-Dinitrotoluene	17A085	2,5-Dinitrotoluene
3,5-Dinitrotoluene	17A086	3,5-Dinitrotoluene
Dinitrotoluenes	17A080	Dinitrotoluenes
Dioctylester o-benzenedicarboxylic acid	08D300	Di-2-ethylhexyl phthalate
Dioctylester phthalic acid	08D300	Di-2-ethylhexyl phthalate
1,4-Dioxane	03B020	1,4-Dioxane
p-Dioxane	03B020	1,4-Dioxane
1,3-Dioxane	03B040	1,3-Dioxane
Dipentylnitrosamine	12A100	N-Nitrosodipentylamine
Diphenyl	15A160	Biphenyl
Diphenyl sulfide	13B060	Diphenyl sulfide

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
Diphenyl thioether	13B060	Diphenyl sulfide
1,2-Diphenylbenzene	15B161	o-Terphenyl
1,3-Diphenylbenzene	15B162	m-Terphenyl
1,4-Diphenylbenzene	15B163	p-Terphenyl
4,4'-Diphenylbiphenyl	15B060	4,4'-Diphenylbiphenyl
Diphenylene oxide	24B020	Dibenzofuran
Diphenylene sulfide	25B060	Dibenzothiophene
4-4'-Diphenylenediamine	10C140	Benzidine
Diphenyleneimine	23C080	Carbazole
Diphenylenemethane	22A020	Fluorene
1,2-Diphenylhydrazine	11B080	1,2-Diphenylhydrazine
Diphenylnitrosamine	12B040	N-Nitrosodiphenylamine
Dipropyl	01A141	n-Hexane
Dipropyl methane	01A181	n-Heptane
Disubstituted, polysubstituted alkyl pyridines	23A140	Disubstituted, polysubstituted alkyl pyridines
Divinyl	01B082	1,3-Butadiene
Divinylene oxide	24A020	Furan
Divinyleneimene	23C020	Pyrrole
DMBA	21B060	7,12-Dimethylbenz(a)anthracene
DMSO	14B020	Dimethyl sulfoxide
n-Dodecane	01A260	n-Dodecane
Dodecanoic acid	08A104	Lauric acid
Dodecylene	01A260	n-Dodecane
Durene	15B203	1,2,4,5-Tetramethylbenzene
Endo-1,7,7-trimethyl bicyclo[2.2.1]heptan-2-ol	05B120	Borneol
Endo-2-bornanol	05B120	Borneol
Endo-2-camphanol	05B120	Borneol
Endo-2-hydroxy camphane	05B120	Borneol
Epichlorhydrin	04A050	Epichlorhydrin
Epihydrin alcohol	06B020	2,3-Epoxy-1-propanol
2,3-Epoxy-1-propanol	06B020	2,3-Epoxy-1-propanol
1,4-Epoxybutane	03A060	Tetrahydrofuran
Erythrene	01B082	1,3-Butadiene
Ethanal	07A040	Acetaldehyde
Ethanamide	08C040	Acetamide
Ethanamine	10A040	Ethylamine
Ethane	01A040	Ethane
1,2-Ethanediamine	10A080	1,2-Diaminoethane
1,2-Ethanediol	06A020	Ethylene glycol
Ethanenitrile	09A020	Acetonitrile
Ethanethiol	13A040	Ethanethiol
Ethanoic acid	08A040	Acetic acid
Ethanol	05A040	Ethanol
Ethanolamine	10A060	Ethanolamine
Ethene	01B020	Ethylene
Ethenylbenezene	15A080	Styrene
Ethine	01C020	Acetylene
Ethyl acetate	08D040	Ethyl acetate
Ethyl acrylate	08D060	Ethyl acrylate
Ethyl adipate	08D200	Diethyl adipate
Ethyl alcohol	05A040	Ethanol
Ethyl aldehyde	07A040	Acetaldehyde
Ethyl benzene	15A060	Ethyl benzene
Ethyl benzol	15A060	Ethyl benzene
Ethyl chloride	02A250	Ethyl chloride
Ethyl cresols	18A160	Ethyl cresols
Ethyl cyanate	09A060	1-Cyanoethane
Ethyl cyanide	09A060	1-Cyanoethane
Ethyl d-carboethoxyvalerate	08D200	Diethyl adipate
Ethyl hydride	01A040	Ethane
Ethyl mercaptan	13A040	Ethanethiol
Ethyl methyl pyridines	23A120	Collidines
Ethyl methylphenols	18A160	Ethyl cresols
1-Ethyl naphthalene	21A043	1-Ethyl naphthalene
2-Ethyl naphthalene	21A044	2-Ethyl naphthalene
Ethyl phosphate	26A020	Triethyl phosphate

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
Ethyl propenoate	08D060	Ethyl acrylate
Ethyl thioalcohol	13A040	Ethanethiol
2-Ethyl-benzo(c)phenanthrene	21B108	2-Ethyl-benzo(c)phenanthrene
6-Ethyl-benzo(c)phenanthrene	21B109	6-Ethyl-benzo(c)phenanthrene
N-Ethyl-ethanamine	10B080	Diethylamine
6-Ethyl-m-cresol	18A161	6-Ethyl-m-cresol
4-Ethyl-o-cresol	18A162	4-Ethyl-o-cresol
2-Ethyl-p-cresol	18A163	2-Ethyl-p-cresol
6-Ethyl-2-methyl phenol	18A161	6-Ethyl-m-cresol
5-Ethyl-2-methylpyridine	23A121	5-Ethyl-2-methylpyridine
4-Ethyl-3-methyl phenol	18A162	4-Ethyl-o-cresol
2-Ethyl-4-methyl phenol	18A163	2-Ethyl-p-cresol
2-Ethyl-4-methyl-1,3-dioxolane	03B060	2-Ethyl-4-methyl-1,3-dioxolane
3-Ethyl-6-methylpyridine	23A121	5-Ethyl-2-methylpyridine
Ethylacetylene	01C061	1-Butyne
Ethylamine	10A040	Ethylamine
bis-2-Ethylbutyl adipic acid ester	08D240	Di-2-ethylbutyl adipate
Ethyldimethylmethane	01A102	Isopentane
Ethylene	01B020	Ethylene
Ethylene chloride	02A260	1-2-Dichloroethane
Ethylene dichloride	02A260	1,2-Dichloroethane
Ethylene glycol	06A020	Ethylene glycol
Ethylene tetrachloride	02B080	Tetrachloroethene
Ethylenediamine	10A080	1,2-Diaminoethane
1,2-Ethylenedicarboxylic acid	08A060	Maleic acid
cis-1,2-Ethylenedicarboxylic acid	08A060	Maleic acid
Ethyleneimine	10B020	Ethyleneimine
1,8-Ethylenenaphthalene	21A100	Acenaphthene
E-Ethylethanamine	10B080	Diethylamine
Ethylethylene	01B061	1-Butene
bis(2-Ethylhexyl)adipate	08D260	Di-2-ethylhexyl adipate
Ethylhydroxy benzenes	18A080	Ethylphenols
Ethylisobutylmethane	01A182	Isoheptane
Ethylmethyl acetaldehyde	07A121	2-Methylbutanal
Ethylmethylamine	10B060	Ethylmethylamine
o-Ethylphenol	18A081	o-Ethylphenol
2-Ethylphenol	18A081	o-Ethylphenol
m-Ethylphenol	18A082	m-Ethylphenol
3-Ethylphenol	18A082	m-Ethylphenol
p-Ethylphenol	18A083	p-Ethylphenol
4-Ethylphenol	18A083	p-Ethylphenol
Ethylphenols	18A080	Ethylphenols
2-Ethylpyridine	23A061	2-Ethylpyridine
3-Ethylpyridine	23A062	3-Ethylpyridine
4-Ethylpyridine	23A063	4-Ethylpyridine
Ethylsulfide	13B040	Diethyl sulfide
Ethyne	01C020	Acetylene
Exo-1,7,7-trimethyl-bicyclo [2.2.2]heptan-2-ol	05B140	Isoborneol
Exo-2-bornanol	05B140	Isoborneol
Exo-2-camphanol	05B140	Isoborneol
Fluoranthene	22B040	Fluoranthene
Fluorene	22A020	Fluorene
2-Fluorenol	18C120	2-Hydroxyfluorene
Fluorotrichloromethane	02A220	Trichlorofluoromethane
Formaldehyde	07A020	Formaldehyde
Formamide	08C020	Formamide
Formic acid	08A020	Formic acid
Formic acid amide	08C020	Formamide
Formosa camphor	07B100	Camphor
Formylamine	08C020	Formamide
Freon 11	02A220	Trichlorofluoromethane
Furan	24A020	Furan
Furfurane	24A020	Furan
Glycidol	06B020	2,3-Epoxy-1-propanol
Glycidyl alcohol	06B020	2,3-Epoxy-1-propanol
Glycol dichloride	02A260	1,2-Dichloroethane

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
Glycolic acid	08B020	Hydroxyacetic acid
Grain alcohol	05A040	Ethanol
Guaiacol	18A060	2-Methoxyphenol
Guaiene	21A082	2,3-Dimethyl naphthalene
Hemimellitene	15B181	1,2,3-Trimethylbenzene
Hendecane	01A242	n-Undecane
n-Heptane	01A181	n-Heptane
Heptanes	01A180	Heptanes
1-Heptene	01B201	1-Heptene
cis-2-Heptene	01B202	cis-2-Heptene
trans-2-Heptene	01B203	trans-2-Heptene
cis-3-Heptene	01B204	cis-3-Heptene
4-Heptene	01B204	cis-3-Heptene
trans-3-Heptene	01B205	trans-3-Heptene
4-Heptene	01B205	trans-3-Heptene
Heptenes	01B200	Heptenes
Heptyl hydride	01A181	n-Heptane
a-Heptylene	01B201	1-Heptene
B-Heptylene	01B202	cis-2-Heptene
g-Heptylene	01B204	cis-3-Heptene
g-Heptylene	01B205	trans-3-Heptene
Hexabenzobenzene	21D100	Coronene
Hexachloro-1,3-butadiene	02B120	Hexachlorobutadiene
Hexachlorobenzene	16A162	Hexachlorobenzene
Hexachlorobutadiene	02B120	Hexachlorobutadiene
Hexachlorocyclohexane	02A380	Hexachlorocyclohexane
1a,2a,3b,4a,5a,6b-Hexachlorocyclohexane	02A380	Hexachlorocyclohexane
Hexachlorocyclopentadiene	02B140	Hexachlorocyclopentadiene
Hexachloroethane	02A320	Hexachloroethane
Hexadecanoic acid	08A122	Palmitic acid
Hexadecyclic acid	08A122	Palmitic acid
Hexahydroaniline	10A160	Cyclohexylamine
Hexahydrobenzene	01A160	Cyclohexane
Hexamethylene	01A160	Cyclohexane
Hexanaphthene	01A160	Cyclohexane
Hexanaphthylene	01B160	Cyclohexene
n-Hexane	01A141	n-Hexane
Hexane dioic acid	08A180	Adipic acid
6-Hexanelactam	08C060	6-Hexanelactam
Hexanes	01A140	Hexanes
Hexanoic acid	08A101	Caproic acid
1-Hexene	01B141	1-Hexene
Hexene	01B141	1-Hexene
cis-2-Hexene	01B142	cis-2-Hexene
trans-2-Hexene	01B143	trans-2-Hexene
cis-3-Hexene	01B144	cis-3-Hexene
trans-3-Hexene	01B145	trans-3-Hexene
Hexenes	01B140	Hexenes
Hexyl hydride	01A141	n-Hexane
Hexylene	01B141	1-Hexene
Hydracrylic acid-b-lactone	08B060	b-Propiolactone
Hydrazobenzene	11B080	1,2-Diphenylhydrazine
Hydrindene	15B020	Indan
Hydroquinol	18B060	1,4-Dihydroxybenzene
Hydroquinone	18B060	1,4-Dihydroxybenzene
2-Hydroxy anisole	18A060	2-Methoxyphenol
4-Hydroxy butanoic acid lactone	08B080	g-Butyrolactone
3-Hydroxy propionic acid lactone	08B060	b-Propiolactone
2-Hydroxy propylamine	10A123	1-Amino-2-propanol
3-Hydroxy-1,2-epoxypropane	06B020	2,3-Epoxy-1-propanol
1-Hydroxy-2-methoxybenzene	18A060	2-Methoxyphenol
1-Hydroxy-2-methyl glutaronitrile	09A100	1,3-Dicyano-1-hydroxybutane
Hydroxyacetic acid	08B020	Hydroxyacetic acid
Hydroxybenzene	18A020	Phenol
2-Hydroxybenzoic acid	08B041	2-Hydroxybenzoic acid
o-Hydroxybenzoic acid	08B041	2-Hydroxybenzoic acid

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
3-Hydroxybenzoic acid	08B042	3-Hydroxybenzoic acid
4-Hydroxybenzoic acid	08B043	4-Hydroxybenzoic acid
p-Hydroxybenzoic acid	08B043	4-Hydroxybenzoic acid
Hydroxybenzoic acids	08B040	Hydroxybenzoic acids
Hydroxybiphenyls	18A100	Phenylphenols
2-Hydroxydibenzofuran	18C140	2-Hydroxydibenzofuran
Hydroxyethanoic acid	08B020	Hydroxyacetic acid
2-Hydroxyethylamine	10A060	Ethanolamine
2-Hydroxyfluorene	18C120	2-Hydroxyfluorene
Hydroxyhydrindene	18C080	Indanols
Hydroxyindan	18C080	Indanols
a-Hydroxynaphthalene	18C020	1-Naphthol
2-Hydroxynaphthalene	18C040	2-Naphthol
2-Hydroxynitrobenzene	20A020	2-Nitrophenol
1-Hydroxyphenanthrene	18C061	1-Hydroxyphenanthrene
2-Hydroxyphenanthrene	18C062	2-Hydroxyphenanthrene
3-Hydroxyphenanthrene	18C063	3-Hydroxyphenanthrene
4-Hydroxyphenanthrene	18C064	4-Hydroxyphenanthrene
9-Hydroxyphenanthrene	18C065	9-Hydroxyphenanthrene
Hydroxyphenanthrenes	18C060	Phenanthrols
o-Hydroxyphenol	18B020	Catechol
2-Hydroxyphenol	18B020	Catechol
1-Hydroxypropane	05A060	1-Propanol
2-Hydroxypropane	05B020	2-Propanol
3-Hydroxypropylene oxide	06B020	2,3-Epoxy-1-propanol
a-Hydroxytoluene	05A140	Benzyl alcohol
Hydroxytoluene	18A040	Cresols
Indan	15B020	Indan
1-Indanol	18C081	1-Indanol
4-Indanol	18C082	4-Indanol
5-Indanol	18C083	5-Indanol
Indanols	18C080	Indanols
Indene	22A010	Indene
11-Indeno(1,2-b)quinoline	23B280	2,3-Benz-4-azafluorene
Indeno(1,2,3-cd)pyrene	22D020	Indeno(1,2,3-cd)pyrene
Indeno(1,2,3-ij)isoquinoline	23B300	Indeno(1,2,3-ij)isoquinoline
Indole	23C040	Indole
Indonaphthene	22A010	Indene
Iodomethane	02A060	Methyl Iodide
IP	22D020	Indeno(1,2,3-cd)pyrene
Isoacetophorone	07B080	Isophorone
Isoamyl acetate	08D143	Isoamyl acetate
sec-Isoamyl alcohol	05B063	3-Methyl-2-butanol
Isoamyl alsohol	05A124	3-Methyl-1-butanol
a-Isoamyl hydride	01A102	Isopentane
Isoborneol	05B140	Isoborneol
Isobutane	01A082	Isobutane
Isobutanol	05A100	Isobutyl alcohol
Isobutene	01B064	Isobutylene
Isobutyl acetate	08D123	Isobutyl acetate
Isobutyl alcohol	05A100	Isobutyl alcohol
Isobutylene	01B064	Isobutylene
Isodurene	15B202	1,2,3,5-Tetramethylbenzene
Isoheptane	01A182	Isoheptane
Isohexane	01A142	Isohexane
Isononane	01A222	Isononane
Isooctane	01A202	Isooctane
Isopentaldehyde	07A122	3-Methylbutanal
Isopentane	01A102	Isopentane
Isophorone	07B080	Isophorone
Isopropanolamine	10A123	1-Amino-2-propanol
2-Isopropoxy propane	03A020	Isopropyl ether
Isopropyl acetate	08D102	Isopropyl acetate
Isopropyl alcohol	05B020	2-Propanol
Isopropyl benzene	15A120	Isopropyl benzene
Isopropyl benzol	15A120	Isopropyl benzene

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
Isopropyl ether	03A020	Isopropyl ether
Isopropyl methyl carbinol	05B063	3-Methyl-2-butanol
Isopropyl-benzo(c)phenanthrene	21B112	Isopropyl-benzo(c)phenanthrene
Isopropylidene chloride	02A344	2,2-Dichloropropane
Isopropylmercaptan	13A062	Propane-2-thiol
Isoquinoline	23B021	Isoquinoline
Isovaleral	07A122	3-Methylbutanal
Isovaleraldehyde	07A122	3-Methylbutanal
Isovaleric aldehyde	07A122	3-Methylbutanal
Lauric acid	08A104	Lauric acid
Leucoline	23B022	Isoquinoline
Lindane	02A380	Hexachlorocyclohexane
2,3-Lutidine	23A141	2,3-Dimethylpyridine
2,4-Lutidine	23A142	2,4-Dimethylpyridine
2,5-Lutidine	23A143	2,5-Dimethylpyridine
2,6-Lutidine	23A144	2,6-Dimethylpyridine
3,4-Lutidine	23A145	3,4-Dimethylpyridine
M.E.K.	07B060	Butanone
Maleic acid	08A060	Maleic acid
Maleinic acid	08A060	Maleic acid
Malenic acid	08A060	Maleic acid
Marsh gas	01A020	Methane
p-Menth-1-en-8-ol	05C060	a-Terpineol
p-Mentha-6,8-dien-2-one	07B181	Carvone (d or 1)
Mercaptobenzene	13A100	Benzenethiol
1-Mercaptopropanol	13A061	Propane-1-thiol
Mesitol	18A181	2,4,6-Trimethyl phenol
Mesitylene	15B183	1,3,5-Trimethylbenzene
Methacrylic acid	08D080	Methyl methacrylate
2-Methaloctane	01A222	Isononane
Methanal	07A020	Formaldehyde
Methanamide	08C020	Formamide
Methane	01A020	Methane
Methane trichloride	02A100	Chloroform
Methanecarboxamide	08C040	Acetamide
Methanethiol	13A020	Methanethiol
Methanoic acid	08A020	Formic acid
Methanol	05A020	Methanol
1-Methoxy-2-nitrobenzene	17B021	1-Methoxy-2-nitrobenzene
1-Methoxy-3-nitrobenzene	17B022	1-Methoxy-3-nitrobenzene
1-Methoxy-4-nitrobenzene	17B023	1-Methoxy-4-nitrobenzene
Methoxyaniline	10C080	Anisidines
m-Methoxyaniline	10C082	m-Anisidine
2-Methoxybiphenyl	03A040	2-Methoxybiphenyl
Methoxynitrobenzenes	17B020	Methoxynitrobenzenes
2-Methoxyphenol	18A060	2-Methoxyphenol
Methyl a-methylacrylate	08D080	Methyl methacrylate
Methyl acetate	08D020	Methyl acetate
Methyl alcohol	05A020	Methanol
Methyl aldehyde	07A020	Formaldehyde
Methyl anilines	10C040	Aminotoluenes
Methyl benzoate	08D160	Methyl benzoate
2-Methyl benzothiazole	23D040	2-Methyl benzothiazole
Methyl bromide	02A020	Methyl bromide
Methyl butene	01B101	1-Pentene
Methyl chloride	02A040	Methyl chloride
Methyl chloroform	02A280	Trichloroethane
Methyl chloromethyl ether	04A020	Chloromethyl methyl ether
4-Methyl chrysene	21B141	4-Methyl chrysenes
5-Methyl chrysene	21B142	5-Methyl chrysene
Methyl chrysenes	21B140	Methyl chrysenes
Methyl cyanide	09A020	Acetonitrile
Methyl diphenyl ether	03A040	2-Methoxybiphenyl
Methyl dithiomethane	13B080	Methyldisulfide
Methyl ester	08D080	Methyl methacrylate
Methyl ester of benzoic acid	08D160	Methyl benzoate

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
1-Methyl ethyl benzene	15A120	Isopropyl benzene
Methyl ethyl ketone	07B060	Butanone
Methyl glycol	06A040	Propylene glycol
Methyl hydride	01A020	Methane
Methyl iodide	02A060	Methyl iodide
Methyl mercaptan	13A020	Methanethiol
Methyl methacrylate	08D080	Methyl methacrylate
Methyl methylacrylate	08D080	Methyl methacrylate
1-Methyl naphthalene	21A041	1-Methyl naphthalene
2-Methyl naphthalene	21A042	2-Methyl napthalene
1-Methyl phenanthrene	21A201	1-Methyl phenanthrene
3-Methyl phenanthrene	21A202	3-Methyl phenanthrene
Methyl phenanthrenes	21A200	Methyl phenanthrenes
Methyl phenyl nitrosamine	12B020	N-Methyl-N-nitrosoaniline
Methyl propyl carbinol	05B061	2-Pentanol
Methyl sulfide	13B020	Dimethyl sulfide
Methyl sulfoxide	14B020	Dimethyl sulfoxide
a-Methyl-a-hydroxy toluene	05B100	1-Phenylethanol
1-Methyl-benzo(c)phenanthrene	21B102	1-Methyl-benzo(c)phenanthrene
2-Methyl-benzo(c)phenanthrene	21B103	2-Methyl-benzo(c)phenanthrene
5-Methyl-benzo(c)phenanthrene	21B104	5-Methyl-benzo(c)phenanthrene
6-Methyl-benzo(c)phenanthrene	21B105	6-Methyl-benzo(c)phenanthrene
7-Methyl-benzo(c)phenanthrene	21B106	7-Methyl-benzo(c)phenanthrene
8-Methyl-benzo(c)phenanthrene	21B107	8-Methyl-benzo(c)phenanthrene
2-Methyl-methyl ester	08D080	Methyl methacrylate
N-Methyl-N-nitrosoaniline	12B020	N-Methyl-N-nitrosoaniline
N-Methyl-N-nitrosobenzenamine	12B020	N-Methyl-N-nitrosoaniline
2-Methyl-1-butanol	05A122	2-Methyl-1-butanol
3-Methyl-1-butanol	05A124	3-Methyl-1-butanol
3-Methyl-1-butanol acetate	08D143	Isoamyl acetate
2-Methyl-1-propanol	05A100	Isobutyl alcohol
Methyl-1,2-benzophenanthrene	21B140	Methyl chrysenes
3-Methyl-2-butanol	05B063	3-Methyl-2-butanol
2-Methyl-2-butanol	05C040	t-Pentanol
1-Methyl-2-chlorobenzene	16A180	2-Chlorotoluene
2-Methyl-2-phenyl propane	15A143	tert-Butyl benzene
2-Methyl-2-phenyl propane	15A143	tert-Butyl benzene
2-Methyl-2-propanol	05C020	t-Butyl alcohol
2-Methyl-4,6-dinitrophenol	20B020	4,6-Dinitro-o-cresol
2-Methyl-5-(1-methylethenyl)-2-cyclohexene-1-one	07B181	Carvone (d or 1)
Methylacetylene	01C040	Propyne
Methylallene	01B081	1,2-Butadiene
Methylamine	10A020	Methylamine
Methylbenzene	15A040	Toluene
Methylbenzene carboxylate	08D160	Methyl benzoate
2-Methylbenzofuran	24A061	2-Methylbenzofuran
3-Methylbenzofuran	24A062	3-Methylbenzofuran
5-Methylbenzofuran	24A063	5-Methylbenzofuran
7-Methylbenzofuran	24A064	7-Methylbenzofuran
Methylbenzofurans	24A060	Methylbenzofurans
a-Methylbenzyl alcohol	05B100	1-Phenylethanol
2-Methylbutanal	07A121	2-Methylbutanal
3-Methylbutanal	07A122	3-Methylbutanal
Methylbutanals	07A120	Methylbutanals
2-Methylbutane	01A102	Isopentane
2-Methylbutyraldehyde	07A121	2-Methylbutanal
a-Methylbutyraldehyde	07A121	2-Methylbutanal
3-Methylbutyraldehyde	07A122	3-Methylbutanal
3-Methylcarbazole	23C101	3-Methylcarbazole
9-Methylcarbazole	23C102	9-Methylcarbazole
Methylcarbazoles	23C100	Methylcarbazoles
Methylcatechol	18A060	2-Methoxyphenol
20-Methylchlolanthrene	21B080	3-Methylcholanthrene
3-Methylchlolanthrene	21B080	3-Methylcholanthrene
Methyldibenzopyrrole	23C100	Methylcarbazoles
Methyldibenzopyrrole	23C101	3-Methylcarbazole

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
9-Methyldibenzopyrrole	23C102	9-Methylcarbazole
Methyldiphenylenimine	23C100	Methylcarbazoles
3-Methyldiphenylenimine	23C101	3-Methylcarbazole
9-Methyldiphenylenimine	23C102	9-Methylcarbazole
Methyldisulfide	13B080	Methyldisulfide
Methylene bichloride	02A080	Methylene chloride
4,4'-Methylene bis(2-chloroaniline)	10C180	4,4'-Methylene bis(2-chloroaniline)
Methylene chloride	02A080	Methylene chloride
Methylene oxide	07A020	Formaldehyde
Methylethylbromoethane	02A362	2-Bromobutane
Methylethylene glycol	06A040	Propylene glycol
2-Methylheptane	01A202	Isooctane
2-Methylhexane	01A182	Isoheptane
Methylhydrazine	11B020	Monomethylhydrazine
2-Methylindole	23C061	2-Methylindole
3-Methylindole	23C062	3-Methylindole
Methylindoles	23C060	Methylindoles
3-Methyllepidine	23B064	3,4-Dimethylquinoline
Methylmethane	01A040	Ethane
Methylnitrobenzenes	17A040	Nitrotoluenes
Methylnitrosophenylamine	12B020	N-Methyl-N-nitrosoaniline
2-Methylpentane	01A142	Isohexane
Methylphenol	18A040	Cresols
Methylphenylcarbinol	05B100	1-Phenylethanol
2-Methylpropane	01A082	Isobutane
2-Methylpropene	01B064	Isobutylene
1-Methylpropyl benzene	15A142	sec-Butyl benzene
1-Methylpropyl benzene	15A142	sec-Butyl benzene
a-Methylpropylethanoate	08D122	sec-Butyl acetate
b-Methylpropylethanoate	08D123	Isobutyl acetate
1-Methylpyrene	21B200	1-Methylpyrene
2-Methylpyridine	23A041	2-Methylpyridine
3-Methylpyridine	23A042	3-Methylpyridine
4-Methylpyridine	23A042	4-Methylpyridine
Methylpyridines	23A040	Picolines
3-Methylquinaldine	23B061	2,3-Dimethylquinoline
6-Methylquinaldine	23B062	2,6-Dimethylquinoline
2-Methylquinoline	23B040	2-Methylquinoline
Methylthiomethane	13B020	Dimethyl sulfide
2-Methylthiophene	25A041	2-Methylthiophene
3-Methylthiophene	25A042	3-Methylthiophene
Methylthiophenes	25A040	Methylthiophenes
Mono-n-propylamine	10A100	1-Aminopropane
Monoalkyl naphthalenes	21A040	Monoalkyl naphthalenes
Monoallyamine	10A110	3-Aminopropene
Monobromomethane	02A020	Methyl Bromide
Monochloroethane	02A250	Ethyl chloride
Monochloromethyl ether	04A020	Chloromethyl methyl ether
Monomethylamine	10A020	Methylamine
Monomethylhydrazine	11B020	Monomethylhydrazine
Monosubstituted alkyl pyridines	23A060	Monosubstituted alkyl pyridines
Morpholine	10B100	Morpholine
Myristic acid	08A121	Myristic acid
Naphthacene	21B020	Naphthacene
a-Naphthacridine	23B200	Benz(c)acridine
Naphthalene	21A020	Naphthalene
1-Naphthalenol	18C020	1-Naphthol
Naphthalin	21A020	Naphthalene
Naphthaline	21A020	Naphthalene
Naphthene	21A020	Naphthalene
Naphtho(1,2-b)furan	24B041	Naphtho(1,2-b)furan
Naphtho(2,1-b)furan	24B042	Naphtho(2,1-b)furan
Naphtho(2,3-b)furan	24B043	Naphtho(2,3-b)furan
Naphtho-1',2':2,3-anthracene	21C020	1,2-Benzonaphthacene
Naphthofurans	24B040	Naphthofurans
1-Naphthol	18C020	1-Naphthol

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
a-Naphthol	18C020	1-Naphthol
2-Naphthol	18C040	2-Naphthol
b-Naphthol	18C040	2-Naphthol
a-Naphthonitrile	09B041	a-Naphthonitrile
1-Naphthonitrile	09B041	a-Naphthonitrile
b-Naphthonitrile	09B042	b-Naphthonitrile
2-Naphthonitrile	09B042	b-Naphthonitrile
Naphthonitriles	09B040	Naphthonitriles
Naphthopyridine	23B140	Benzo(f)quinoline
b-Naphthoquinoline	23B140	Benzo(f)quinoline
a-Naphthoquinoline	23B160	Benzo(h)quinoline
b-Naphthyl hydroxide	18C040	2-Naphthol
1-Naphthylamine	10C200	1-Aminonaphthalene
a-Naphthylamine	10C200	1-Aminonaphthalene
2-Naphthylamine	10C220	2-Aminonaphthalene
b-Naphthylamine	10C220	2-Aminonaphthalene
Naphthyleneethylene	21A100	Acenaphthene
2,3-Naptho-2,3-phenanthrene	21C020	1,2-Benzonaphthacene
Necatorina	02A240	Carbon Tetrachloride
Neopentane	01A103	Neopentane
Neopentyl alcohol	05A123	2,2-Dimethyl-1-propanol
Nitroanisoles	17B020	Methoxynitrobenzenes
Nitrobenzene	17A020	Nitrobenzene
4-Nitrobiphenyl	17A060	4-Nitrobiphenyl
p-Nitrobiphenyl	17A060	4-Nitrobiphenyl
p-Nitrochlorobenzene	17B060	1-Chloro-4-nitrobenzene
4-Nitrodiphenyl	17A060	4-Nitrobiphenyl
2-Nitrophenol	20A020	2-Nitrophenol
o-Nitrophenol	20A020	2-Nitrophenol
3-Nitrophenol	20A040	3-Nitrophenol
m-Nitrophenol	20A040	3-Nitrophenol
4-Nitrophenol	20A060	4-Nitrophenol
p-Nitrophenol	20A060	4-Nitrophenol
Nitrophenyl methyl ethers	17B020	Methoxynitrobenzenes
N-Nitroso-N-dipropylamine	12A060	N-Nitrosodipropylamine
N-Nitroso-N-methylaniline	12B020	N-Methyl-N-nitrosoaniline
N-Nitrosodiethylamine	12A040	N-Nitrosodiethylamine
N-Nitrosodiisopropylamine	12A080	N-Nitrosodiisopropylamine
Nitrosodiisopropylamine	12A080	N-Nitrosodiisopropylamine
N-Nitrosodimethylamine	12A020	N-Nitrosodimethylamine
N-Nitrosodipentylamine	12A100	N-Nitrosodipentylamine
N-Nitrosodiphenylamine	12B040	N-Nitrosodiphenylamine
N-Nitrosodipropylamine	12A060	N-Nitrosodipropylamine
Nitrosomethylaniline	12B020	N-Methyl-N-nitrosoaniline
N-Nitrosophenylamine	12B020	N-Methyl-N-nitrosoaniline
2-Nitrotoluene	17A041	2-Nitrotoluene
3-Nitrotoluene	17A042	3-Nitrotoluene
4-Nitrotoluene	17A043	4-Nitrotoluene
Nitrotoluenes	17A040	Nitrotoluenes
Nitrous diisopropylamide	12A080	N-Nitrosodiisopropylamine
Nitrous diphenylamide	12B040	N-Nitrosodiphenylamine
Nitrous dipropyl amide	12A060	N-Nitrosodipropylamine
n-Nonane	01A221	n-Nonane
Nonanes	01A220	Nonanes
Nonyl alcohol	05B080	2,6-Dimethyl-4-heptanol
Octadecanoic acid	08A123	Stearic acid
cis-9-Octadecanoic acid	08A140	Oleic acid
n-Octane	01A201	n-Octane
Octanes	01A200	Octanes
Octanoic acid	08A102	Caprylic acid
Octyl phthalate	08D300	Di-2-ethylhexyl phthalate
Oleic acid	08A140	Oleic acid
2-Oxetanone	08B060	b-Propiolactone
2-Oxobovane	07B100	Camphor
Oxole	24A020	Furan
Oxybenzene	18A020	Phenol

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
1,1'-Oxybis (2-chloroethane)	04B080	2,2'-Dichlorodiethyl ether
Oxybis[chloromethane]	04B020	1,1'-Dichloromethyl ether
2,2'-Oxybis[propane]	03A020	Isopropyl ether
Palmitic acid	08A122	Palmitic acid
b-Parvolone	23A146	2,3,4,6-Tetramethylpyridine
PCB's	16A220	Polychlorinated biphenyls
Pentachlorophenol	19A060	Pentachlorophenol
Pentamethylene	01A120	Cyclopentane
n-Pentane	01A101	n-Pentane
Pentanes	01A100	Pentanes
Pentanoic acid	08A080	Valeric acid
n-Pentanol	05A121	n-Pentanol
1-Pentanol	05A121	n-Pentanol
2-Pentanol	05B061	2-Pentanol
3-Pentanol	05B062	3-Pentanol
t-Pentanol	05C040	t-Pentanol
Pentanols, (primary)	05A120	Pentanols, (primary)
Pentanols, (secondary)	05B060	Pentanols, (secondary)
1-Pentene	01B101	1-Pentene
cis-2-Pentene	01B102	cis-2-Pentene
trans-2-Pentene	01B103	trans-2-Pentene
Pentenes	01B100	Pentenes
2-Pentyl acetate	08D142	sec-Amyl acetate
t-Pentyl alcohol	05C040	t-Pentanol
1-Pentylene	01B101	1-Pentene
Perchlorobenzene	16A162	Hexachlorobenzene
Perchlorocyclopentadiene	02B140	Hexachlorocyclopentadiene
Perchloroethane	02A320	Hexachloroethane
Perchlcroethylene	02B080	Tetrachloroethene
Perchloromethane	02A240	Carbon Tetrachloride
Perchloromethanethiol	13A140	Perchloromethanethiol
Perchloromethyl mercaptan	13A140	Perchloromethanethiol
Periethylenenaphthalene	21A100	Acenaphthene
Perylene	21C140	Perylene
Phenanthrene	21A180	Phenanthrene
Phenanthridine	23B120	Phenanthridine
Phenanthro(9,10-b)furan	24B080	Phenanthro(9,10-b)furan
Phenanthrols	18C060	Phenanthrols
Phenanthrylene methane	22B080	Cyclopenta(def)phenanthrene
Phene	15A020	Benzene
Phenethyl alcohol	05A160	Phenethyl alcohol
B-Phenethyl alcohol	05A160	Phenethyl alcohol
a-Phenethyl alcohol	05B100	1-Phenylethanol
Phenic acid	18A020	Phenol
Phenol	18A020	Phenol
o-Phenyl anisole	03A040	2-Methoxybiphenyl
Phenyl benzoate	08D180	Phenyl benzoate
Phenyl bromide	16A040	Bromobenzene
1-Phenyl butane	15A141	n-Butyl benzene
2-Phenyl butane	15A142	sec-Butyl benzene
2-Phenyl butane	15A142	sec-Butyl benzene
Phenyl chloride	16A020	Chlorobenzene
Phenyl cyanide	09B020	Benzonitrile
Phenyl formic acid	08A160	Benzoic acid
Phenyl hydroxide	18A020	Phenol
Phenyl mercaptan	13A100	Benzenethiol
Phenyl methanol	05A140	Benzyl alcohol
Phenyl methyl ketone	07B120	Acetophenone
1-Phenyl propane	15A100	Propyl benzene
Phenyl pyridines	23A080	Phenyl pyridines
2-Phenyl pyridines	23A081	2-Phenyl pyridines
3-Phenyl pyridines	23A082	3-Phenyl pyridines
4-Phenyl pyridines	23A083	4-Phenyl pyridines
Phenyl sulfide	13B060	Diphenyl sulfide
Phenylaldehyde	07A140	Benzaldehyde
Phenylamine	10C020	Aniline

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
p-Phenylaniline	10C120	4-Aminobiphenyl
Phenylbenzene	15A160	Biphenyl
Phenylcarbinol	05A140	Benzyl alcohol
p-Phenylenediamine	10C100	1,4-Diaminobenzene
2,3-o-Phenylenepyrene	22D020	Indeno(1,2,3-cd)pyrene
Phenylethane	15A060	Ethyl benzene
2-Phenylethanol	05A160	Phenethyl alcohol
1-Phenylethanol	05B100	1-Phenylethanol
1-Phenylethanone	07B120	Acetophenone
Phenylethylene	15A080	Styrene
Phenylhydride	15A020	Benzene
Phenylic acid	18A020	Phenol
Phenylmethane	15A040	Toluene
Phenylmethyl alcohol	05A140	Benzyl alcohol
1-Phenylnaphthalene	21A061	1-Phenylnaphthalene
2-Phenylnaphthalene	21A062	2-Phenylnaphthalene
Phenylnaphthalenes	21A060	Phenylnaphthalenes
o-Phenylphenol	18A101	o-Phenylphenol
p-Phenylphenol	18A102	p-Phenylphenol
m-Phenylphenol	18A103	m-Phenylphenol
Phenylphenols	18A100	Phenylphenols
2-Phenylpropane	15A120	Isopropyl benzene
Phenylsulfonic acid	14A020	Benzenesulfonic acid
Phenylthiobenzene	13B060	Diphenyl sulfide
Phthalate esters	08D280	Phthalate esters
Phthalic acid	08A200	Phthalic acid
o-Phthalic acid	08A200	Phthalic acid
Picene	21C160	Picene
Picolines	23A040	Picolines
Picramic acid	20A080	2-Amino-4,6-dinitrophenol
Picraminic acid	20A080	2-Amino-4,6-dinitrophenol
Picric acid	20A120	2,4,6-Trinitrophenol
Polyalkyl phenols (MW greater than 135)	18A180	Polyalkyl phenols (MW greater than 135)
Polychlorinated benzenes	16A160	Polychlorinated benzenes
Polychlorinated Biphenyls (PCB's)	16A220	Polychlorinated biphenyls (PCB's)
Prehnitene	15B201	1,2,3,4-Tetramethylbenzene
Propaldehyde	07A080	Propionaldehyde
Propanal	07A080	Propionaldehyde
Propanamine	10A100	1-Aminopropane
Propane	01A060	Propane
Propane	01B040	Propylene
Propane-1-thiol	13A061	Propane-1-thiol
Propane-2-thiol	13A062	Propane-2-thiol
1,2-Propanediol	06A040	Propylene glycol
2-Propanenitrile	09A040	Acrylonitrile
Propanenitrile	09A060	1-Cyanoethane
1-Propanethiol	13A061	Propane-1-thiol
2-Propanethiol	13A062	Propane-2-thiol
Propanethiols	13A060	Propanethiols
Propanoic acid-3-hydroxy lactone	08B060	b-Propiolactone
1-Propanol	05A060	1-Propanol
2-Propanol	05B020	2-Propanol
B-Propanolamine	10A121	2-Amino-1-propanol
Propanolamines	10A120	Propanolamines
Propanolide	08B060	b-Propiolactone
2-Propanone	07B020	Acetone
Propenal	07A060	Acrolein
2-Propene-1-amine	10A110	3-Aminopropene
2-Propenoic acid ethyl ether	08D060	Ethyl acrylate
Propine	01C040	Propyne
b-Propiolactone	08B060	b-Propiolactone
Propionaldehyde	07A080	Propionaldehyde
Propionitrile	09A060	1-Cyanoethane
b-Propiono lactone	08B060	b-Propiolactone
n-Propyl acetate	08D101	n-Propyl acetate
Propyl acetates	08D100	Propyl acetates

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
n-Propyl alcohol	05A060	1-Propanol
Propyl aldehyde	07A080	Propionaldehyde
Propyl benzene	15A100	Propyl benzene
Propyl cyanide	09A080	Butyronitrile
Propyl nitrosamine	12A060	N-Nitrosodipropylamine
n-Propyl-benzo(c)phenanthrene	21B111	n-Propyl-benzo(c)phenanthrene
Propylacetic acid	08A080	Valeric acid
n-Propylamine	10A100	1-Aminopropane
Propylene	01B040	Propylene
Propylene chloride	02A342	1,2-Dichloropropane
Propylene dichloride	02A342	1,2-Dichloropropane
Propylene glycol	06A040	Propylene glycol
Propylethylene	01B101	1-Pentene
Propylidene chloride	02A341	1,1-Dichloropropane
Propylidene dichloride	02A341	1,1-Dichloropropane
Propylmercaptan	13A061	Propane-1-thiol
Di-n-propylnitrosamine	12A060	N-Nitrosodipropylamine
4-n-Propylpyridine	23A064	4-n-Propylpyridine
Propyne	01C040	Propyne
Pseudobutyl benzene	15A143	tert-Butyl benzene
Pseudobutyl benzene	15A143	tert-Butyl benzene
Pseudobutylene	01B062	cis-2-Butene
Pseudocumene	15B182	1,2,4-Trimethylbenzene
Pyrene	21B180	Pyrene
Pyridine	23A020	Pyridine
a-Pyridylbenzene	23A081	2-Phenyl pyridines
a-Pyridylbenzene	23A081	2-Phenyl pyridines
b-Pyridylbenzene	23A082	3-Phenyl pyridines
g-Pyridylbenzene	23A083	4-Phenyl pyridines
Pyrocatechol	18B020	Catechol
Pyrogallic acid	18B080	1,2,3-Trihydroxybenzene
Pyrogallol	18B080	1,2,3-Trihydroxybenzene
Pyrrole	23C020	Pyrrole
p,p'-Quaterphenyl	15B060	4,4'-Diphenylbiphenyl
Quinaldine	23B040	2-Methylquinoline
Quinol	18B060	1,4-Dihydroxybenzene
Quinoline	23B021	Quinoline
Quinolines	23B020	Quinolines
Resorcinol	18B040	1,3-Dihydroxybenzene
Rubbing alcohol	05B020	2-Propanol
Salicylic acid	08B041	2-Hydroxybenzoic acid
Saturated Long Chain Acids (MW:116-201)	08A100	Saturated Long Chain Acids (MW:116-201)
Saturated Long Chain Acids(MW:228-285)	08A120	Saturated Long Chain Acids(MW:228-285)
Secondary butylamine	10A142	2-Aminobutane
Skatole	23C062	3-Methylindole
Stearic acid	08A123	Stearic acid
Styrene	15A080	Styrene
Styrolene	15A080	Styrene
Sulfinylbis[methane]	14B020	Dimethyl sulfoxide
Tar camphor	21A020	Naphthalene
Telone	02B103	cis-1,3-Dichloropropene
o-Terphenyl	15B161	o-Terphenyl
m-Terphenyl	15B162	m-Terphenyl
p-Terphenyl	15B163	p-Terphenyl
Terphenyls	15B160	Terphenyls
a-Terpineol	05C060	a-Terpineol
Tertiary butylamine	10A143	2-Amino-2-methylpropane
Tetracene	21B020	Naphthacene
1,1,3,3-Tetrachloro-2-propanone	07C020	Tetrachloroacetone
Tetrachloroacetone	07C020	Tetrachloroacetone
1,1,2,2-Tetrachloroethane	02A300	1,1,2,2-Tetrachloroethane
Tetrachloroethene	02B080	Tetrachloroethene
Tetrachloroethylene	02B080	Tetrachloroethene
Tetrachloromethane	02A240	Carbon Tetrachloride
Tetradecanoic acid	08A121	Myristic acid
n-Tetradecoic acid	08A121	Myristic acid

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
Tetrahydro-1,4-oxazine	10B100	Morpholine
3a,7,7,7a-Tetrahydro-4,7-methanoindene	01B220	Dicyclopentadiene
3,4,5,6-Tetrahydrobenzene	01B160	Cyclohexene
Tetrahydrobenzene	01B160	Cyclohexene
Tetrahydrofuran	03A060	Tetrahydrofuran
Tetrahydronaphthalene	15B120	Tetrahydronaphthalene
Tetralin	15B120	Tetrahydronaphthalene
Tetraline	15B120	Tetrahydronaphthalene
1,2,3,4-Tetramethylbenzene	15B201	1,2,3,4-Tetramethylbenzene
1,2,3,5-Tetramethylbenzene	15B202	1,2,3,5-Tetramethylbenzene
1,2,4,5-Tetramethylbenzene	15B203	1,2,4,5-Tetramethylbenzene
Tetramethylbenzenes	15B200	Tetramethylbenzenes
Tetramethylmethane	01A103	Neopentane
Tetramethylsuccinonitrile	09A120	Tetramethylsuccinonitrile
Tetraphenyl	15B060	4,4'-Diphenylbiphenyl
Tetrole	24A020	Furan
1-1'-Thiobis[benzene]	13B060	Diphenyl sulfide
1-1'-Thiobisethane	13B040	Diethyl sulfide
Thiobismethane	13B020	Dimethyl sulfide
Thioethylether	13B040	Diethyl sulfide
Thiofuran	25A020	Thiophene
Thionaphthene	25B040	Benzo(b)thiophene
Thiophene	25A020	Thiophene
Thiophenol	13A100	Benzenethiol
2,3-Thioxene	25A061	2,3-Dimethylthiophene
2,4-Thioxene	25A062	2,4-Dimethylthiophene
a,a-Thioxene	25A063	2,5-Dimethylthiophene
TMSN	09A120	Tetramethylsuccinonitrile
Toluene	15A040	Toluene
a-Toluenol	05A140	Benzyl alcohol
Toluidines	10C040	Aminotoluenes
Toluol	15A040	Toluene
o-Toluquinaldine	23B120	2,8-Dimethylquinoline
o-Tolyl chloride	16A180	2-Chlorotoluene
Toxilic acid	08A060	Maleic acid
Tri-m-tolyl phosphate	26B043	Tri-m-tolyl phosphate
Tri-o-cresyl phosphate	260B42	Tri-o-tolyl phosphate
Tri-o-tolyl phosphate	26B041	Tri-o-tolyl phosphate
Tri-p-tolyl phosphate	26B042	Tri-p-tolyl phosphate
Tribenzylene benzene	22D040	Tribenzylene benzene
Tribromomethane	02A160	Bromoform
1,2,4-Trichlorobenzene	16A161	1,2,4-Trichlorobenzene
Trichloroethane	02A280	Trichloroethane
1,1,1-Trichloroethane	02A280	Trichloroethane
1,1,2-Trichloroethane	02A290	1,1,2-Trichloroethane
B-Trichloroethane	02A290	1,1,2-Trichloroethane
Trichloroethylene	02B070	Trichloroethylene
Trichlorofluoromethane	02A220	Trichlorofluoromethane
Trichloromethane	02A100	Chloroform
Trichloromethanethiol	13A140	Perchloromethanethiol
Trichloromonofluoromethane	02A220	Trichlorofluoromethane
2,4,6-Trichlorophenol	19A050	2,4,6-Trichlorophenol
Tricresol phosphate	26B040	Tritolyl phosphate
Triethyl phosphate	26A020	Triethyl phosphate
1,2,3-Trihydroxybenzene	18B080	1,2,3-Trihydroxybenzene
Trimethyl and tetramethyl thiophenes	25A080	Trimethyl and tetramethyl thiophenes
Trimethyl carbinol	05C020	t-Butyl alcohol
2,4,6-Trimethyl phenol	18A181	2,4,6-Trimethyl phenol
3,5,5-Trimethyl-2-cyclohexene-1-one	07B080	Isophorone
a,a,4-Trimethyl-3-cyclohexene-1-methanol	05C060	a-Terpineol
1,2,3-Trimethylbenzene	15B181	1,2,3-Trimethylbenzene
1,2,4-Trimethylbenzene	15B182	1,2,4-Trimethylbenzene
1,3,5-Trimethylbenzene	15B183	1,3,5-Trimethylbenzene
Trimethylbenzenes	15B180	Trimethylbenzenes
1,7,7-Trimethylbicyclo[2.2.1]heptan-2-one	07B100	Camphor
Trimethylbromomethane	02A363	2-Bromoisobutane

COMPOUND/ELEMENT	CATEGORY	PREFERRED NAME
Trimethylene chloride	02A343	1,3-Dichloropropane
Trimethylmethane	01A082	Isobutane
2,2,4-Trimethylpentane	01A202	Isooctane
Trimethylphenyl methane	15A143	tert-Butyl benzene
Trimethylphenyl methane	15A143	tert-Butyl benzene
Trimethylpyridines	23A120	Collidines
2,3,5-Trimethylthiophene	25A081	2,3,5-Trimethylthiophene
2,4,6-Trinitrophenol	20A120	2,4,6-Trinitrophenol
Triorthocresol phosphate	26B041	Tri-o-tolyl phosphate
Triphenyl phosphate	26B020	Triphenyl phosphate
Triphenylene	21B160	Triphenylene
Tritolyl phosphate	26B040	Tritolyl phosphate
Truxene	22D040	Tribenzylene benzene
TSN	09A120	Tetramethylsuccinonitrile
n-Undecane	01A242	n-Undecane
Unsym-trichlorobenzene	16A161	1,2,4-Trichlorobenzene
Unsymmetrical dimethylhydrazine	11B040	N,N-Dimethylhydrazine
Valerianic acid	08A080	Valeric acid
Valeric acid	08A080	Valeric acid
Vinyl benzene	15A080	Styrene
Vinyl chloride	02B020	Vinyl chloride
Vinyl cyanide	09A040	Acrylonitrile
Vinylidene chloride	02B060	1,1-Dichloroethene
Wood alcohol	05A020	Methanol
o-Xylene	15B081	o-Xylene
m-Xylene	15B082	m-Xylene
p-Xylene	15B083	p-Xylene
o-Xylene chloride	16B041	1,2-bis (Chloromethyl) benzene
m-Xylene chloride	16B042	1-3-bis (Chloromethyl) benzene
p-Xylene chloride	16B043	1,4-bis (Chloromethyl) benzene
Xylenes	15B080	Xylenes
2,3-Xylenol	18A141	2,3-Xylenol
2,4-Xylenol	18A142	2,4-Xylenol
2,5-Xylenol	18A143	2,5-Xylenol
2,6-Xylenol	18A144	2,6-Xylenol
3,5-Xylenol	18A145	3,5-Xylenol
3,4-Xylenol	18A146	3,4-Xylenol
Xylenols	18A140	Xylenols
2,3-Xylidine	10C061	2,3-Xylidine
2,4-Xylidine	10C062	2,4-Xylidine
2,5-Xylidine	10C063	2,5-Xylidine
2,6-Xylidine	10C064	2,6-Xylidine
3,4-Xylidine	10C065	3,4-Xylidine
3,5-Xylidine	10C066	3,5-Xylidine
Xylidines	10C060	Dimethylanilines
Xylol	15B080	Xylenes

MOLECULAR FORMULA INDEX FOR ORGANIC COMPOUNDS ADDRESSED BY MEG'S

CBr_2Cl_2	02A180
CCl_2F_2	02A200
CCl_3F	02A220
CCl_4	02A240
$CHBrCl_2$	02A120
$CHBr_2Cl$	02A140
$CHBr_3$	02A160
$CHCL_3$	02A100
$CHCl_3S$	13A140
CH_2Cl_2	02A080
CH_2O	07A020
CH_2O_2	08A020
CH_2N_2	11A020
CH_3Br	02A020
CH_3Cl	02A040
CH_3I	02A060
CH_3	08C020
CH_4	01A020
CH_4O	05A020
CH_4S	13A020
CH_5N	10A020
CH_6N_2	11B020
$C_2Cl_2F_2$	02B090
C_2Cl_4	02B080
C_2HCl_3	02B070
C_2Cl_6	02A320
C_2H_2	01C020
$C_2H_2Cl_2$	02B040
$C_2H_2Cl_2$	02B060
$C_2H_2Cl_4$	02A300
C_2H_3Cl	02B020
$C_2H_3Cl_3$	02A280
$C_2H_3Cl_3$	02A290
C_2H_3N	09A020
C_2H_4	01B020
$C_2H_4O_2$	08A040
$C_2H_4Cl_2$	02A260
$C_2H_4Cl_2O$	04B020
C_2H_4O	07A040
$C_2H_4O_3$	08B020
C_2H_5Cl	02A250
C_2H_5ClO	04A020
C_2H_5N	10B020
C_2H_5NO	08C040
C_2H_6	01A040
$C_2H_6N_2O$	12A020
C_2H_6O	05A040
$C_2H_6S_2$	13B080
C_2H_6SO	14B020
$C_2H_6O_2$	06A020
C_2H_6S	13A040
C_2H_6S	13B020
C_2H_7N	10A040
C_2H_7N	10B040
C_2H_7NO	10A060
$C_2H_8N_2$	10A080
$C_2H_8N_2$	11B040
$C_2H_8N_2$	11B060
$C_3H_2Cl_4O$	07C020
C_3H_3N	09A040
C_3H_4	01C040
$C_3H_4Cl_2$	02B100
C_3H_4O	07A060
$C_3H_4O_2$	08B060
C_3H_5ClO	04A040
C_3H_5ClO	04A050
C_3H_5ClO	04A060
C_3H_5N	09A060

INDEX (Continued)

C_3H_6 01B040
$C_3H_6Cl_2$ 02A340
C_3H_6O 07B020
C_3H_6O 07A080
$C_3H_6O_2$ 06B020
$C_3H_6O_2$ 08D020
C_3H_7N 10A110
C_3H_7ClO 04A080
C_3H_7ClO 04A100
C_3H_8 01A060
C_3H_8O 05A020
C_3H_8O 05A060
C_3H_8O 05B020
$C_3H_8O_2$ 06A040
C_3H_8S 13A060
C_3H_9N 10A100
C_3H_9N 10B060
C_3H_9NO 10A120
C_4Cl_6 02B120
C_4H_4O 24A020
$C_4H_4O_4$ 08A060
C_4H_4S 25A020
C_4H_5N 23C020
C_4H_6 01B080
C_4H_6 01C060
$C_4H_6O_3$ 08B060
C_4H_7ClO 04A140
C_4H_7N 09A080
C_4H_8 01B060
$C_4H_8Cl_2O$ 04B040
$C_4H_8Cl_2O$ 04B060
$C_4H_8Cl_2O$ 04B080
C_4H_8O 03A060
C_4H_8O 07A100
C_4H_8O 07B060
$C_4H_8O_2$ 03B020
$C_4H_4O_2$ 03B040
$C_4H_8O_2$ 08B040
C_4H_9Br 02A360
C_4H_9ClO 04A120
C_4H_9NO 10B100
C_4H_{10} 01A080
$C_4H_{10}O$ 05A080
$C_4H_{10}O$ 05A100
$C_4H_{10}O$ 05A080
$C_4H_{10}N_2O$ 12A040
$C_4H_{10}O$ 05C020
$C_4H_{10}O$ 05B040
$C_4H_{10}S$ 13A080
$C_4H_{10}S$ 13B040
$C_4H_{11}N$ 10A140
$C_4H_{11}N$ 10B080
C_5H_4ClN 23A100
C_5H_5N 23A020
C_5Cl_6 02B140
C_5H_6 01B120
C_5H_6S 25A040
$C_5H_8O_2$ 08D060
$C_5H_8O_2$ 08D080
C_5H_{10} 01B100
C_5H_{10} 01A120
$C_5H_{10}O$ 07A120
$C_5H_{10}O_2$ 08A080
$C_5H_{10}O_2$ 08D100
C_5H_{12} 01A100
$C_5H_{12}O$ 05A120
$C_5H_{12}O$ 05B060
$C_5H_{12}O$ 05C040

INDEX (Continued)

C_6Cl_6	16A162
$C_6H_nCl_n$	16A160
C_6HCl_5O	19A060
$C_6H_3Cl_3$	16A161
$C_6H_3N_2O_7$	20A120
C_6H_4BrCl	16A080
$C_6H_4Br_2$	16A060
$C_6H_4ClNO_2$	17B040
$C_6H_4ClNO_2$	17B060
$C_6H_4Cl_2$	16A100
$C_6H_4Cl_2$	16A120
$C_6H_4Cl_2$	16A140
$C_6H_4Cl_2O$	19A040
$C_6H_4N_2O_5$	20A100
C_6H_5Br	16A040
C_6H_5Cl	16A020
C_6H_5ClO	19A020
$C_6H_5NO_2$	17A020
$C_6H_5NO_3$	20A020
$C_6H_5NO_3$	20A040
$C_6H_5NO_3$	20A060
$C_6H_5N_3O_5$	20A080
C_6H_6	15A020
$C_6H_6Cl_6$	02A380
C_6H_6O	18A020
$C_6H_6O_2$	18B020
$C_6H_6O_2$	18B040
$C_6H_6O_2$	18B060
$C_6H_6O_3$	18B080
$C_6H_6SO_3$	14A020
C_6H_6	13A100
C_6H_7N	10C020
C_6H_7N	23A040
C_6H_8	01B180
$C_6H_8N_2$	10C100
$C_6H_8N_2O$	09A100
C_6H_8S	25A060
C_6H_{10}	01B160
$C_6H_{10}O_2$	08A101
$C_6H_{10}O_4$	08A180
$C_6H_{11}NO$	08C060
C_6H_{12}	01A160
C_6H_{12}	01B140
$C_6H_{12}O_2$	03B060
$C_6H_{12}O_2$	08D120
$C_6H_{12}Cl_2O$	04B100
$C_6H_{13}ClO$	04A160
$C_6H_{13}N$	10A160
$C_6H_{13}NO_2$	08B100
C_6H_{14}	01A140
$C_6H_{14}N_2O$	12A060
$C_6H_{14}N_2O$	12A080
$C_6H_{14}O$	03A020
$C_6H_{15}O_4P$	26A020
C_7H_5N	09B020
C_7H_5NS	23D020
$C_7H_6N_2O_4$	17A080
$C_7H_6N_2O_5$	20B020
$C_7H_6N_2O_5$	20B040
C_7H_6O	07A140
$C_7H_6O_2$	08A160
$C_7H_6O_3$	08B040
C_7H_7Cl	16A180
C_7H_7Cl	16B020
C_7H_7ClO	19B020
$C_7H_7NO_2$	17A040

INDEX (Continued)

$C_7H_7NO_3$	17B020
C_7C_8	15A040
$C_7H_8N_2O$	12B020
C_7H_8O	05A140
C_7H_8O	18A040
$C_7H_8O_2$	18A060
C_7H_9N	10C040
C_7H_9N	23A141
C_7H_9N	23A142
C_7H_9N	23A143
C_7H_9N	23A144
C_7H_9N	23A145
C_7H_9N	23A061
C_7H_9N	23A062
C_7H_9N	23A063
C_7H_9NO	10C080
$C_7H_{10}S$	25A081
C_7H_{14}	01B200
$C_7H_{14}O_2$	08D140
C_7H_{16}	01A180
C_8H_6O	24A040
$C_8H_6O_4$	08A200
C_8H_6S	25B040
$C_8H_6S_2$	25B020
C_8H_7N	23C040
C_8H_7NS	23D040
$C_8H_8Cl_2$	16B040
$C_8H_8O_2$	07B120
$C_8H_8O_2$	08D160
C_8H_{10}	15B080
C_8H_{10}	15A060
$C_8H_{10}N$	05A160
$C_8H_{10}O$	05B100
$C_8H_{10}O$	18A080
$C_8H_{10}N$	18A140
$C_8H_{11}N$	10C060
$C_8H_{11}N$	10D020
$C_8H_{11}N$	23A120
$C_8H_{11}N$	23A064
C_8H_{12}	15A080
$C_8H_{12}N_2$	09A120
$C_8H_{16}Cl_2O$	04B120
$C_8H_{16}O_2$	08A102
$C_8H_{17}Cl$	02A400
C_8H_{18}	01A200
C_9H_7N	23B020
C_9H_8	22A010
C_9H_8O	24A060
C_9H_9N	23C060
C_9H_{10}	15B020
$C_9H_{10}O$	18C080
C_9H_{12}	15B180
C_8H_{12}	15A100
C_9H_{12}	15A120
C_9H_{12}	15B180
$C_9H_{12}O$	18A160
$C_9H_{12}O$	18A181
$C_9H_{13}N$	23A146
$C_9H_{14}O$	07B080
C_9H_{20}	01A220
$C_9H_{20}O$	05B080
$C_{10}H_7Cl$	16A200
$C_{10}H_8$	21A020
$C_{10}H_8O$	18C020
$C_{10}H_8O$	18C040
$C_{10}H_9N$	10C200
$C_{10}H_9N$	10C220
$C_{10}H_9N$	23B040

INDEX (Continued)

$C_{10}H_{10}$ 15B140
$C_{10}H_{10}O_4$ 08D281
$C_{10}H_{12}$ 01B220
$C_{10}H_{12}$ 15B120
$C_{10}H_{14}$ 15A140
$C_{10}H_{14}$ 15B101
$C_{10}H_{14}$ 15B102
$C_{10}H_{14}$ 15B103
$C_{10}H_{14}$ 15B200
$C_{10}H_{14}O$ 07B181
$C_{10}H_{16}O$ 07B100
$C_{10}H_{16}O$ 07B182
$C_{10}H_{18}O$ 05B120
$C_{10}H_{18}O$ 05B140
$C_{10}H_{18}O$ 05C060
$C_{10}H_{18}O_4$ 08D200
$C_{10}H_{20}O_2$ 08A103
$C_{10}H_{22}$ 01A240
$C_{10}H_{22}N_2O$ 12A100
$C_{11}H_7N$ 09B040
$C_{11}H_7O_2$ 18C140
$C_{11}H_9N$ 23A080
$C_{11}H_{10}$ 21A040
$C_{11}H_{10}$ 21A042
$C_{11}H_{11}N$ 23B060
$C_{11}H_{24}$ 01A242
$C_{12}Cl_n$ 16A220
$C_{12}H_8$ 21A100
$C_{12}H_8O$ 24B020
$C_{12}H_8O$ 24B040
$C_{12}H_8S$ 25B060
$C_{12}H_9BrO$ 04A200
$C_{12}H_9ClO$ 04A180
$C_{12}H_9N$ 23C080
$C_{12}H_9NO_2$ 17A060
$C_{12}H_{10}$ 15A160
$C_{12}H_{10}$ 21A100
$C_{12}H_{10}ClN$ 10C160
$C_{12}H_{10}N_2O$ 12B040
$C_{12}H_{10}O$ 18A100
$C_{12}H_{10}O$ 18C100
$C_{12}H_{10}O_2$ 18A120
$C_{12}H_{10}S$ 13B060
$C_{12}H_{11}N$ 10C120
$C_{12}H_{12}$ 21A043
$C_{12}H_{12}$ 21A044
$C_{12}H_{12}$ 21A080
$C_{12}H_{12}N_2$ 10C140
$C_{12}H_{12}N_2$ 11B080
$C_{12}H_{14}O_4$ 08D282
$C_{12}H_{18}$ 15B104
$C_{12}H_{18}$ 15B105
$C_{12}H_{26}$ 01A260
$C_{13}H_9ClO_2$ 07C040
$C_{13}H_9N$ 23B080
$C_{13}H_9N$ 23B120
$C_{13}H_9N$ 23B140
$C_{13}H_9N$ 23B160
$C_{13}H_{10}$ 22A020
$C_{13}H_{10}O$ 18C120
$C_{13}H_{10}O_2$ 08D180
$C_{13}H_{11}N$ 23B100
$C_{13}N_{11}N$ 23C100
$C_{13}H_{12}$ 22A040
$C_{13}H_{12}Cl_2N_2$ 10C180
$C_{13}H_{12}O$ 03A040
$C_{14}H_8C_8S_2$ 14A040
$C_{14}H_{10}$ 21A140

INDEX (Continued)

$C_{14}H_{10}$	21A180
$C_{14}H_{10}O$	18C060
$C_{14}H_{10}S$	13A120
$C_{14}H_{15}N_3$	11A040
$C_{14}H_{22}$	15B106
$C_{14}H_{22}O$	18A182
$C_{14}H_{26}O_4$	08D220
$C_{14}H_{28}O_2$	08A121
$C_{15}H_9N$	23B300
$C_{15}H_{10}$	22B080
$C_{15}H_{12}$	21A201
$C_{15}H_{24}O$	18A183
$C_{16}H_{10}$	22B040
$C_{16}H_{10}$	21B180
$C_{16}H_{10}O$	24B060
$C_{16}H_{10}O$	24B080
$C_{16}H_{10}O$	24B100
$C_{16}H_{10}S$	25B080
$C_{16}H_{11}N$	23C120
$C_{16}H_{11}N$	23B280
$C_{16}H_{12}$	21A060
$C_{16}H_{14}$	21A160
$C_{16}H_{22}O_4$	08D283
$C_{16}H_{32}O_2$	08A122
$C_{17}H_{11}N$	23B180
$C_{17}H_{11}N$	23B200
$C_{17}H_{12}$	21B200
$C_{17}H_{12}$	22B020
$C_{17}H_{12}$	22B060
$C_{17}H_{12}O$	07B160
$C_{18}H_{12}$	21B040
$C_{18}H_{12}$	21B101
$C_{18}H_{12}$	21B120
$C_{18}H_{14}$	15B160
$C_{18}H_{14}$	21B220
$C_{18}H_{15}O_4P$	26B020
$C_{18}H_{34}O_2$	08A140
$C_{18}H_{34}O_4$	08D240
$C_{18}H_{36}O_2$	08A123
$C_{19}H_{14}$	21B102
$C_{19}H_{14}$	21B103
$C_{19}H_{14}$	21B104
$C_{19}H_{14}$	21B105
$C_{19}H_{14}$	21B106
$C_{19}H_{14}$	21B107
$C_{19}H_{14}$	21B140
$C_{19}H_{20}O_4$	08D320
$C_{20}H_{12}$	22C020
$C_{20}H_{12}$	22C040
$C_{20}H_{12}$	22C080
$C_{20}H_{12}$	21C100
$C_{20}H_{12}$	21C120
$C_{20}H_{12}$	21C140
$C_{20}H_{13}N$	23C140
$C_{20}H_{13}N$	23C160
$C_{20}H_{13}N$	23C180
$C_{20}H_{16}$	21B060
$C_{20}H_{17}$	21B108
$C_{20}H_{17}$	21B109
$C_{21}H_{13}N$	23B220
$C_{21}H_{13}N$	23B240
$C_{21}H_{13}N$	23B260
$C_{21}H_{14}$	22C060
$C_{21}H_{16}$	21B080
$C_{21}H_{18}$	21B10A
$C_{21}H_{18}$	21B10B
$C_{21}H_{21}O_4P$	26B040
$C_{22}H_{12}$	21D080

INDEX (Continued)

$C_{22}H_{12}$ 22D020
$C_{22}H_{14}$ 21C020
$C_{22}H_{14}$ 21C040
$C_{22}H_{14}$ 21C060
$C_{22}H_{14}$ 21C080
$C_{22}H_{14}$ 21C160
$C_{22}H_{42}O_2$ 08D260
$C_{24}H_{12}$ 21D100
$C_{24}H_{14}$ 21D020
$C_{24}H_{14}$ 21D040
$C_{24}H_{14}$ 21D060
$C_{24}H_{20}$ 15B060
$C_{24}H_{38}O_4$ 08D300
$C_{27}H_{18}$ 22D040

APPENDIX A

MEG CHARTS AND BACKGROUND INFORMATION SUMMARIES

Appendix A of the MEG's report consists of background information summaries and MEG charts for organic compounds included in the MEG's Master List and is contained in this volume and in Volume III. The charts and summaries are arranged by MEG's categories. Categories 1 through 12 are included in Volume III; Categories 13-26 are in this volume (the distinguishing characteristics of each of the MEG's categories are discussed in Volume IA, Appendix B).

Charts and summaries contained in this appendix address 586 organic chemicals. At the beginning of each subcategory of compounds, a brief tabulation is provided giving the number of compounds addressed in the subcategory, the number of suspected carcinogens or teratogens included, the number of compounds without numerical MEG's, and the specific Consent Decree compounds included. A separate reference list is supplied for each subcategory allowing the user to ascertain quickly if a particular reference has been used in the preparation of the summaries for a compound group. The consolidated alphabetized bibliography for the background information summaries is given in Appendix F, contained in Volume IA.

An alphabetical index of preferred names and synonyms for the organic MEG compounds and a molecular formula index are included in the front matter of each volume of Appendix A.

The methodology developed for establishing Multimedia Environmental Goals as outlined in Volume IA has been applied in the preparation of the background information summaries and MEG charts contained in this appendix.

CATEGORY 13

THIOLS, SULFIDES, AND DISULFIDES

SUBCATEGORY: 13A - Thiols

Summary of Subcategory

Total number of compounds in subcategory	9
number of parent compounds with subspecies	2
number of subspecies	4
Number of parent compounds with no MEG values	1
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

Consent Decree compounds included in subcategory: None

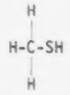
CATEGORY: 13A

WLN: SH1

METHANETHIOL: CH_4S (methyl mercaptan).

A colorless gas; odor of rotten cabbage. 13A020

STRUCTURE:



$$H-\overset{\displaystyle H}{\underset{\displaystyle H}{C}}-SH$$

PROPERTIES:

Molecular wt: 48.1; mp: -123.1; bp: 7.6; d: 0.868; vap. d: 1.66; vap. press.: 2 atmos at 26.1°; slightly soluble in hot water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Methanethiol is found in coal tar. It is also formed catalytically from methanol and hydrogen sulfide.

The odor of methanethiol is stronger and more unpleasant than that of hydrogen sulfide (ref. 1). The odor threshold level is reported as 0.0021 ppm (ref. 2). Methanethiol is flammable and emits SO_2 on burning. It will also react with hot water or steam (ref. 3).

TOXIC PROPERTIES, HEALTH EFFECTS:

There is a close toxicologic similarity between methanethiol and hydrogen sulfide. Acute toxicity is characterized by respiratory effects, including respiratory paralysis and edema (ref. 1).

LD_{50} (subcutaneous, mouse): 2.4 mg/kg.

LC_{Lo} (inhalation, rat): 10,000 ppm.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 1 mg/m^3 (0.5 ppm).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $1.0 \times 10^3\ \mu g/m^3$ (0.5 ppm)

Water, Health: $15 \times 1.0 \times 10^3 = 1.5 \times 10^4\ \mu g/\ell$

Land, Health:

Air, Ecology:

Water, Ecology:

Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 1/420 = 2.4\ \mu g/m^3$

$EPC_{AH1a} = 0.5/420 = 0.001$ ppm

$EPC_{WH1} = 15 \times 2.4 = 36\ \mu g/\ell$

$EPC_{WH2} = 13.8 \times 1 = 13.8\ \mu g/\ell$

MULTIMEDIA ENVIRONMENTAL GOALS

13A020
METHANETHIOL

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.0E3 (0.5)		2.4 (0.001)		
Water, $\mu g/l$ (ppm Wt)			1.5E4		13.8		
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

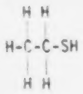
	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			2.4 (0.001)		
Water, $\mu g/l$ (ppm Wt)			14		
Land, $\mu g/g$ (ppm Wt)					

CATEGORY: 13A

WLN: SH2

ETHANETHIOL: C_2H_6S (ethyl mercaptan, ethyl thioalcohol).
A colorless liquid; penetrating, garlic odor. 13A040

STRUCTURE:



$$\begin{array}{c} H\ \ H \\ H-C-C-SH \\ H\ \ H \end{array}$$

PROPERTIES:

Molecular wt: 62.13; mp: -147; bp: 36.2; d: 0.83907;
vap. d: 2.14; vap. press.: 400 mm at 17.7°; slightly soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

The most significant characteristic of ethanethiol is the intense odor. The odor threshold is also reported as 1 ppb (ref. 2).

Rural background concentration is reported as 1 ppb (ref. 4). This is equivalent to 2.5 μg/m^3.

Ethanethiol reacts with water, steam, acid, or heat to produce toxic and flammable vapors, such as SO_x (ref. 3).

TOXIC PROPERTIES, HEALTH EFFECTS:

The lowest concentration of ethanethiol resulting in a toxic response in a human is reported as 4 ppm. This concentration resulted in effects to the central nervous system (ref. 5). Hydrogen sulfide is considered to be 10 times more toxic than ethanethiol (ref. 1).

Only slight acute toxicity for ethanethiol is indicated by animal responses.

LC_{50} (inhalation, rat): 4,420 ppm (ref. 1).

LD_{50} (oral, rat): 682 mg/kg.

Aquatic toxicity: 0.24 mg/ℓ is reported to cause tainting in fish (ref. 10).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 1 mg/m^3 (0.5 ppm) (based on intense odor).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 1.0×10^3 μg/m^3 (0.5 ppm)
Water, Health: $15 \times 1.0 \times 10^3 = 1.5 \times 10^4$ μg/ℓ
Land, Health: $0.2 \times 1.5 \times 10^4 = 3.0 \times 10^3$ μg/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 1/420 = 2.4$ μg/m^3
$EPC_{AH1a} = 0.5/420 = 0.001$ ppm
$EPC_{WH1} = 15 \times 2.4 = 36$ μg/ℓ
$EPC_{WH2} = 13.8 \times 1 = 13.8$ μg/ℓ
$EPC_{LH} = 0.2 \times 13.8 = 3$ μg/g

$EPC_{WE2} = 240$ μg/ℓ (to prevent tainting)
$EPC_{LE} = 0.2 \times 240 = 48$ μg/g

40<

13A040
ETHANETHIOL

EMISSION LEVEL GOALS	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.0E3 (0.5)		2.4 (0.001)		2.5
Water, $\mu g/l$ (ppm Wt)			1.5E4		13.8	240	
Land, $\mu g/g$ (ppm Wt)			3.0E3		3	48	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			2.4 (0.001)		
Water, $\mu g/l$ (ppm Wt)			14	240	
Land, $\mu g/g$ (ppm Wt)			3	48	

CATEGORY: 13A

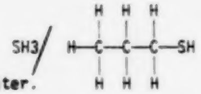
WLN:

PROPANETHIOLS: C_3H_8S 13A060

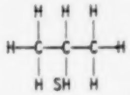
PROPANE-1-THIOL: (1-mercaptopropanol, propylmercaptan, 1-propanethiol). A liquid with an offensive odor. 13A061

PROPANE-2-THIOL: (2-propanethiol, isopropylmercaptan). A liquid. 13A062

STRUCTURE:



(propane-1-thiol)



(propane-2-thiol)

PROPERTIES:

propane-1-thiol: mol. wt: 76.17; mp: -113.3; bp: $67\text{-}8^{760}$; d: 0.8411^{20}; vap. press: 100 mm at 15.3°C; slightly soluble in water.

propane-2-thiol: mol. wt: 76.17; mp: -130.54; bp: 52.56; d: 0.8143; slightly soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Odor is probably the most significant quality of the propanethiols. Odor threshold in air is reported to be 0.075 to 0.75 ppb or 0.23 to 2.3 $\mu g/m^3$ (ref. 11). A faint odor is detectable in water at a concentration of 0.075 $\mu g/\ell$ (ref. 11). Background level is expected to be below the odor threshold of 0.23 $\mu g/m^3$.

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxic properties are probably similar to the properties of the other low molecular weight thiols. Most thiols are not highly toxic. Animal studies indicate the propanethiols are less toxic than ethanethiol.

LD_{50} (oral, rat): 1,790 mg/kg for propane-1-thiol (ref. 5).

LC_{50} (inhalation, rat): 7,300 ppm/4 hr, (mouse): 4010 ppm/4 hr (ref. 5).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$45 \times 1,790 = 8.06 \times 10^4$ $\mu g/m^3$	Air, Ecology:
Water, Health:	$15 \times 8.06 \times 10^4 = 1.21 \times 10^6$ $\mu g/l$	Water, Ecology:
Land, Health:	$0.2 \times 1.21 \times 10^6 = 2.4 \times 10^5$ $\mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 1,790 = 191.5$ $\mu g/m^3$

$EPC_{AH3} = 0.081 \times 1,790 = 145$ $\mu g/m^3$

$EPC_{WH1} = 15 \times 145 = 2,175$ $\mu g/l$

$EPC_{WH2} = 0.4 \times 1,790 = 716$ $\mu g/l$

$EPC_{LH} = 0.2 \times 716 = 143$ $\mu g/g$

13A060
PROPANETHIOLS

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			8.06E4		145		<0.23
Water, $\mu g/l$ (ppm Wt)			1.21E6		716		0.075
Land, $\mu g/g$ (ppm Wt)			2.42E5		143		

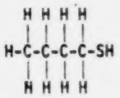
*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			145		
Water, $\mu g/l$ (ppm Wt)			716		
Land, $\mu g/g$ (ppm Wt)			143		

CATEGORY: 13A

WLN: SH4

STRUCTURE:



$$H_3C\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}SH$$

n-BUTANETHIOL: $C_4H_{10}S$ (n-butyl mercaptan, 1-butanethiol, n-butyl-thioalcohol). 13A080

A colorless, mobile liquid; heavy skunk-like odor.

PROPERTIES:

Molecular wt: 90.18; mp: -116; bp: 98; d: 0.8365; vap. d: 3.1; slightly soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

The odor threshold for butanethiol is reported ranging from 0.001 to 0.0001 ppm; the odor is readily noticeable at 0.1 to 1 ppm (ref. 1). This compound occurs infamously in skunk oil (ref. 6).

Natural background concentration in air is expected to be below the odor threshold level of 1 ppb or 3.6 $\mu g/m^3$.

TOXIC PROPERTIES, HEALTH EFFECTS:

Odor is the most significant characteristic of n-butanethiol.

Toxicity is believed to be slight and similar to the toxicity of the other thiols. The lowest concentration to have a toxic effect on a human is 10 mg/m^3 for 3 hours (ref. 5).

LC_{50} (inhalation, rat): 4,020 ppm for 4 hrs.

LD_{50} (oral, rat): 1,500 mg/kg.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 1.5 mg/m^3 (0.5 ppm).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 1.5×10^3 $\mu g/m^3$ (0.5 ppm)

Water, Health: $15 \times 1.5 \times 10^3 = 2.25 \times 10^4$ $\mu g/\ell$

Land, Health: $0.2 \times 2.25 \times 10^4 = 4.5 \times 10^3$ $\mu g/g$

Air, Ecology:

Water, Ecology:

Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 1.5/420 = 3.6\ \mu g/m^3$

$EPC_{AH1a} = 0.5/420 = 0.001$ ppm

$EPC_{WH1} = 15 \times 3.6 = 54\ \mu g/\ell$

$EPC_{WH2} = 13.8 \times 1.5 = 21\ \mu g/\ell$

$EPC_{LH} = 0.2 \times 21 = 4\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

13A080
n-BUTANETHIOL

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)			1.5E3 (0.5)		3.6 (0.001)		<3.6
Water, μg/l (ppm Wt)			2.25E4		21		
Land, μg/g (ppm Wt)			4.5E3		4		

*To be multiplied by dilution factor

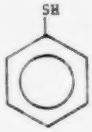
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)			3.6 (0.001)		
Water, μg/l (ppm Wt)			21		
Land, μg/g (ppm Wt)			4		

CATEGORY: 13A

BENZENETHIOL: C_6H_5SH (thiophenol, phenyl mercaptan, mercaptobenzene). 13A100
A colorless liquid with a repulsive odor.

WLN: SHR

STRUCTURE:



PROPERTIES:

Molecular wt: 110.18; mp: -14.8; bp: 168.7^{760}; d: 1.0766_4^{20}; vap. press: 10 mm at 56°C; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzenethiol is used in mosquito larvacide (ref. 3).

Odor threshold is reported as low as 0.0002 ppm or 0.9 $\mu g/m^3$ (ref. 11). Odor is detectable in water as low as 0.000062 mg/ℓ (ref. 11). Natural background concentrations may be expected to be below odor threshold levels.

TOXIC PROPERTIES, HEALTH EFFECTS:

Benzenethiol is reported to cause severe dermatitis, headache, and dizziness (ref. 3). Toxicity appears to be greater than the low molecular weight aliphatic thiols.

LD_{50} (oral, rat): 46 mg/kg (ref. 5).
LC_{50} (inhalation, rat): 33 ppm/4 hr (ref. 5).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Benzenethiol is the subject of a NIOSH Criteria Document. The NIOSH recommendation for occupational exposure to benzenethiol is a ceiling of 0.5 mg/m^3 (0.1 ppm)(ref. 12).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 5×10^2 $\mu g/m^3$ (0.1 ppm)	Air, Ecology:
Water, Health: $15 \times 5 \times 10^2 = 7.5 \times 10^3$ $\mu g/l$	Water, Ecology:
Land, Health: $0.2 \times 7.3 \times 10^3 = 1.5 \times 10^3$ $\mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 0.5/420 = 1.19\ \mu g/m^3$

$EPC_{AH1a} = 0.1/420 = 0.0002$ ppm

$EPC_{WH1} = 15 \times 1.19 = 17.9\ \mu g/l$

$EPC_{WH2} = 13.8 \times 0.5 = 7\ \mu g/\ell$

$EPC_{LH} = 0.2 \times 7 = 1.4\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

X
13A100
BENZENETHIOL

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			5.0E2 (0.1)		1.2 (0.0002)		0.9
Water, μg/l (ppm Wt)			7.5E3		7		0.062
Land, μg/g (ppm Wt)			1.5E3		1.4		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			1.2 (0.0002)		
Water, μg/l (ppm Wt)			7		
Land, μg/g (ppm Wt)			1.4		

CATEGORY: 13A

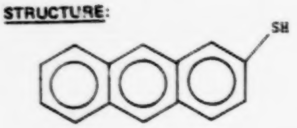
ANTHRACENETHIOLS: $C_{14}H_{10}S$ 13A120

2-ANTHRACENETHIOL: pale yellow crystals. 13A121

9-ANTHRACENETHIOL: pale yellow crystals. 13A122

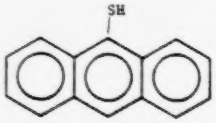
WLN:

STRUCTURE:



PROPERTIES:

	mol.wt.	mp.	solubility in water
2-anthracenethiol	210.29	220	slight
9-anthracenethiol	210.29	90-91	slight



NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Anthracenthiols are used in the manufacturing of dyes and the vulcanization of rubber (ref. 9).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for anthracenethiols are not available at this time.

There is no evidence to indicate that this compound is carcinogenic, although the parent structure, anthracene, has produced tumors in animals when administered in very high dosages.

Analogy with naphthalene would indicate toxicity is not increased by the thiol function. Thiols may also be compared with alcohols. Data for naphthalene compounds are given below:

Compound (ref. 5)	LD_{50} (oral, rat) mg/kg	LD_{Lo} (mouse) mg/kg
Naphthalene	1,780	150 (intraperitoneal)
1-Naphthol	2,590	
2-Naphthol	2,420	100 (subcutaneous)
2-Naphthalenethiol	-	200 (intraperitoneal)

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

13A120
ANTHRACENETHIOLS

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

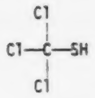
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

CATEGORY: 13A

PERCHLOROMETHANETHIOL: $CHCl_3S$ (trichloromethanethiol, perchloromethyl mercaptan). A gas. 13A140

WLN: SHXGGG

STRUCTURE:



$$Cl-\overset{\displaystyle Cl}{\underset{\displaystyle Cl}{C}}-SH$$

PROPERTIES:

Molecular wt: 151.43

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

TOXIC PROPERTIES, HEALTH EFFECTS:

Perchloromethanethiol is considered a highly toxic and irritating gas (ref. 1).

Human death has resulted from exposure to 483 ppm of perchloromethanethiol for 10 minutes (ref. 5). Eye effects were experienced at levels of 45 ppm (ref. 5).

LD_{50} (oral, rat): 83 mg/kg

LD_{Lo} (inhalation, mouse): 58 ppm for 10 minutes; (cat): 58 ppm for 15 minutes (58 ppm = 357 mg/m^3).

Evidence of carcinogenicity: Perchloromethanethiol has produced cancer in rats when administered by inhalation intermittently at 15 mg/m^3 over 68 weeks. The EPA/NIOSH ordering number for the compound is 4121. However, since a dosage cannot be determined for the data given, an adjusted ordering number cannot be calculated.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.8 mg/m^3 (0.1 ppm).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$10^3 \times 0.8 = 800\ \mu g/m^3$ (0.1 ppm)	Air, Ecology:
Water, Health:	$15 \times 800 = 1.2 \times 10^4\ \mu g/l$	Water, Ecology:
Land, Health:		Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 0.8/420 = 1.90\ \mu g/m^3$

$EPC_{AH1a} = 0.1/420 = 2.38 \times 10^{-4}$ ppm

$EPC_{WH1} = 15 \times 1.90 = 28.5\ \mu g/l$

$EPC_{WH2} = 13.8 \times 0.8 = 11.04\ \mu g/l$

XX
13A140
PERCHLOROMETHANETHIOL

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			8.0E2 (0.1)		1.90 (0.0002)		
Water, $\mu g/l$ (ppm Wt)			1.2E4		11.04		
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects†
Air, $\mu g/m^3$ (ppm Vol)			1.90 (0.0002)		
Water, $\mu g/l$ (ppm Wt)			11		
Land, $\mu g/g$ (ppm Wt)					

†Compound has caused cancer in rats via inhalation.

REFERENCES: CATEGORY 13A

Thiols, Sulfides, and Disulfides - Thiols

1. American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values for Substances in Workroom Air with Supplements, Third Edition. American Conference of Governmental Industrial Hygienists, Cincinnati, OH (1974).

2. Billings, C. E., Technological Sources of Air Pollution. Industrial Pollution, N. I. Sax, Ed., Van Nostrand Rheinhold Co., New York, NY (1974).

3. Sax, N. I., Ed. Dangerous Properties of Industrial Materials, Fourth Edition. Van Nostrand Reinhold Co., New York, NY (1975).

4. Wagoner, D. Compilation of Ambient Trace Substances. Draft of Report Prepared by Research Triangle Institute Under Contract No. 68-02-1325 for U.S. Environmental Protection Agency. Available from W. G. Tucker, Project Officer, IERL-EPA, Research Triangle Park, N.C. (1976).

5. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

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7. Jacobson, J. S., and A. C. Hill, Eds. Recognition of Air Pollution Injury to Vegetation: A Pictorial Atlas. Informative Report No. 1. TR-70 Agricultural Committee-Air Pollution Control Administration. Herbich and Held Printing Co., Pittsburgh, PA (1970).

8. Bond, R. G., C. P. Straub, and R. Prober, Eds. Handbook of Environmental Control. Vol. 1: Air Pollution. The Chemical Rubber Co., Cleveland, OH (1972).

9. Chemical Abstracts, Vol. 54, p. 6176i, 1960.

10. National Academy of Sciences, National Academy of Engineering. Water Quality Criteria 1972. National Academy of Sciences, Washington, DC. EPA-R3-73-033 (1973).

11. Verschueren, K. Handbook of Environmental Data on Organic Chemicals. Van Nostrand Rheinhold Company, NY (1977).

12. National Institute for Occupational Safety and Health. Criteria for a Recommended Standard: Occupational Exposure to Benzenethiol. National Institute for Occupational Safety and Health. U.S. Department of Health, Education, and Welfare (1978).

CATEGORY 13

THIOLS, SULFIDES, AND DISULFIDES

SUBCATEGORY: 13B - Sulfides, Disulfides

Summary of Subcategory

Total number of compounds in subcategory	4
number of parent compounds with subspecies	0
number of subspecies	0
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

Consent Decree compounds included in subcategory: None

CATEGORY: 13B

WLN: 1S1

DIMETHYL SULFIDE: C_2H_6S (methyl sulfide, methylthiomethane, thiobismethane).
A colorless liquid with a disagreeable odor. 13B020

STRUCTURE:

$H_3C{-}S{-}CH_3$

PROPERTIES:

Molecular wt: 62:13; mp: -98.27; 37.3^{760}; d:0.8483;
vap. d: 2.14; vap. press: 420 mm at 20°C; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Dimethyl sulfide is used as a solvent for anhydrous mineral salts (ref. 1). It is formed by the distillation of potassium methyl sulfate (ref. 1).
The odor threshold for dimethyl sulfide is 0.001 ppm or 2.5 $\mu g/m^3$ (ref. 2).
In water, dimethyl sulfide at 0.0011 mg/ℓ has a faint odor (ref. 7).
Natural background levels may be expected to be lower than odor thresholds.

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{50} (oral, rat): 535 mg/kg (ref. 3).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$45 \times 535 = 2.41 \times 10^4$ $\mu g/m^3$	Air, Ecology:	
Water, Health:	$15 \times 2.41 \times 10^4 = 3.6 \times 10^5$ $\mu g/l$	Water, Ecology:	
Land, Health:	$0.2 \times 3.6 \times 10^5 = 7.2 \times 10^4$ $\mu g/g$	Land, Ecology:	

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 535 = 57$ $\mu g/m^3$

$EPC_{AH3} = 0.081 \times 535 = 43$ $\mu g/m^3$

$EPC_{WH1} = 15 \times 43 = 645$ $\mu g/l$

$EPC_{WH2} = 0.4 \times 535 = 214$ $\mu g/l$

$EPC_{LH} = 0.2 \times 214 = 43$ $\mu g/g$

13B020
DIMETHYL SULFIDE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.41E4		43		<2.5
Water, $\mu g/l$ (ppm Wt)			3.6E5		214		<1.1
Land, $\mu g/g$ (ppm Wt)			7.2E4		43		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			43		
Water, $\mu g/l$ (ppm Wt)			214		
Land, $\mu g/g$ (ppm Wt)			43		

CATEGORY: 13B

DIETHYL SULFIDE: $C_4H_{10}S$ (ethylsulfide, 1,1'-thio(bis)ethane, thioethylether).
A colorless liquid with a garlic-like odor. 13B040

WLN:

STRUCTURE:

$CH_3CH_2—S—CH_2CH_3$

PROPERTIES:

Molecular wt: 90.19; mp: -103.19; bp: 92.1^{760}; d: 0.8362^{20}_{4};
vap.d: 3.11; vap. press: 100 mm at 35°C; solubility in water: 3,130 mg/ℓ at 20°C.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Diethylsulfide is used as a solvent for anhydrous mineral salts; in plating baths for coating metals with gold or silver. It is formed by distillation of sodium ethyl sulfate (ref. 1).

When heated to decomposition, or on contact with acid or acid fumes, diethylsulfide emits fumes of sulfur oxides (ref. 4)

Odor threshold in air is reported at 0.59 ppb or 2.2 μg/m³ (ref. 7).

Water containing 0.25 μg/ℓ exhibits a faint odor (ref. 7).

Natural background levels may be expected to be lower than odor thresholds.

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for diethyl sulfide are not available at this time. Its properties are likely to be similar to those of diethyl disulfide, LD_{50} (oral, rat) reported as 2,030 mg/kg. (ref. 3). There is no evidence to indicate that the compound is highly toxic.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

*MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 200 = 9 \times 10^4$ μg/m³

Water, Health: $15 \times 9 \times 10^4 = 1.35 \times 10^6$ μg/ℓ

Land, Health: $0.2 \times 1.35 \times 10^6 = 2.7 \times 10^5$ μg/g

Air, Ecology:

Water, Ecology:

Land, Ecology:

*ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 2000 = 214$ μg/m³

$EPC_{AH3} = 0.081 \times 2000 = 162$ μg/m³

$EPC_{WH1} = 15 \times 162 = 2{,}430$ μg/ℓ

$EPC_{WH2} = 0.4 \times 2000 = 800$ μg/ℓ

$EPC_{LH} = 0.2 \times 800 = 160$ μg/g

*Based on estimated LD_{50} by analogy with diethyldisulfide.

MULTIMEDIA ENVIRONMENTAL GOALS

13B040
DIETHYL SULFIDE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on † Health Effects	Based on Ecological Effects	Based on † Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			9.0E4		162		<2.2
Water, $\mu g/l$ (ppm Wt)			1.35E6		800		<0.25
Land, $\mu g/g$ (ppm Wt)			2.7E5		160		

*To be multiplied by dilution factor

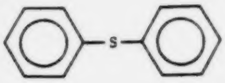
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects †	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			162		
Water, $\mu g/l$ (ppm Wt)			800		
Land, $\mu g/g$ (ppm Wt)			160		

†Based on estimated LD_{50} by analogy with diethyldisulfide.

CATEGORY: 13B
DIPHENYL SULFIDE: $(C_6H_5)_2S$ (phenyl sulfide, 1,1'-thiobis [benzene], dipheny1 thioether, phenylthiobenzene). A colorless liquid. 13B060

WLN: RSR

STRUCTURE:



PROPERTIES:

Molecular wt: 186.28; mp: -25.9; bp: 296; d: 1.1126^{20}_{4}; vap. press: 1 mm at 96.1°C; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

The odor threshold for diphenyl sulfide is 4.7 ppb (ref. 2) to 2.1 ppb or 16 $\mu g/m^3$ (ref. 7).

Water containing 0.048 $\mu g/\ell$ exhibits a faint odor (ref. 7).

Natural background levels may be expected to be lower than odor thresholds.

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{50} (oral, rat): 2,140 mg/kg (ref. 3).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$45 \times 2{,}140 = 9.63 \times 10^4$ $\mu g/m^3$	Air, Ecology:	
Water, Health:	$15 \times 9.63 \times 10^4 = 1.44 \times 10^6$ $\mu g/l$	Water, Ecology:	
Land, Health:	$0.2 \times 1.44 \times 10^6 = 2.9 \times 10^5$ $\mu g/g$	Land, Ecology:	

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 2{,}140 = 229$ $\mu g/m^3$

$EPC_{AH3} = 0.081 \times 2{,}140 = 173.3$ $\mu g/m^3$

$EPC_{WH1} = 15 \times 173.3 = 2{,}600$ $\mu g/l$

$EPC_{WH2} = 0.4 \times 2{,}140 = 856$ $\mu g/l$

$EPC_{LH} = 0.2 \times 856 = 170$ $\mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

13B060
DIPHENYL SULFIDE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			9.63E4		173.3		<16
Water, $\mu g/l$ (ppm Wt)			1.44E6		856		<0.048
Land, $\mu g/g$ (ppm Wt)			2.9E5		170		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			173.3		
Water, $\mu g/l$ (ppm Wt)			856		
Land, $\mu g/g$ (ppm Wt)			170		

CATEGORY: 13B
METHYLDISULFIDE: $C_2H_6S_2$ (dimethyl disulfide, methyl dithiomethane).
A liquid. 13B080

WLN:

STRUCTURE:

$CH_3—S—S—CH_3$

PROPERTIES:

Molecular wt: 94.2; mp: -84.72; bp: 109.7^{760}; d: 1.0625^{20}_{4}
insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Methyldisulfide has been reported in samples taken from finished drinking waters (ref. 5). It occurs in coal gas (ref. 6). The compound emits sulfur oxide fumes when heated to decomposition.
Odor threshold in air is reported as 1 ppb or 5 $\mu g/m^3$, 5 $\mu g/\ell$ in water (ref. 7).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for methyldisulfide are not available at this time. Its properties are likely to be similar to those of diethyldisulfide, LD_{50} (oral, rat) reported as 2,030 mg/kg (ref. 3). There is no evidence to indicate that the compound is highly toxic. The no-effect level in rats is reported as 100 ppm, 20 x 6 hours (ref. 7). 100 ppm is equivalent to 383 mg/m^3.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

*MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 2000 = 9 \times 10^4$ $\mu g/m^3$

Water, Health: $15 \times 9 \times 10^4 = 1.35 \times 10^6$ $\mu g/\ell$

Land, Health: $0.2 \times 1.35 \times 10^6 = 2.7 \times 10^5$ $\mu g/g$

Air, Ecology:

Water, Ecology:

Land, Ecology:

*ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 2000 = 214$ $\mu g/m^3$

$EPC_{AH3} = 0.081 \times 2000 = 162$ $\mu g/m^3$

$EPC_{WH1} = 15 \times 162 = 2{,}430$ $\mu g/\ell$

$EPC_{WH2} = 0.4 \times 2000 = 800$ $\mu g/\ell$

$EPC_{LH} = 0.2 \times 800 = 160$ $\mu g/g$

*Based on estimated LD_{50} by analogy with diethyldisulfide.

MULTIMEDIA ENVIRONMENTAL GOALS

13B080
METHYL DISULFIDE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on † Health Effects	Based on Ecological Effects	Based on † Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			9.0E4		162		< 5
Water, $\mu g/l$ (ppm Wt)			1.35E6		800		< 5
Land, $\mu g/g$ (ppm Wt)			2.7E5		160		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects†	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			162		
Water, $\mu g/l$ (ppm Wt)			800		
Land, $\mu g/g$ (ppm Wt)			160		

†Based on estimated LD_{50} by analogy with diethyldisulfide.

REFERENCES: CATEGORY 13B

Thiols, Sulfides, and Disulfides - Sulfides, Disulfides

1. Windholz, M., Ed. The Merck Index: An Encyclopedia of Chemicals and Drugs, Ninth Edition. Merck & Co., Inc., Rahway, NJ (1976).
2. Billings, C. E., Technological Sources of Air Pollution. Industrial Pollution, N. I. Sax, Ed., Van Nostrand Rheinhold Co., New York, NY (1974).
3. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).
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5. Shackelford, W. M., and L. H. Keith. Frequency of Organic Compounds Identified in Water. EPA Publication No. 600/4-76-062, December 1976.
6. Mezey, E. J., S. Singh, and D. W. Hissong. Fuel Contaminants Vol. I Chemistry. EPA Publication No. EPA 600/2-76-177a. 1976.
7. Verschueren, K. Handbook of Environmental Data on Organic Chemicals. Van Nostrand Rheinhold Company, NY (1977).

CATEGORY 14

SULFONIC ACIDS, SULFOXIDES

SUBCATEGORY: 14A - Sulfonic Acids

Summary of Subcategory

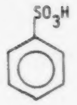
Total number of compounds in subcategory	5
number of parent compounds with subspecies	1
number of subspecies	4
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

Consent Decree compounds included in subcategory: None

CATEGORY: 14A

WLN: WSQR

STRUCTURE:



BENZENESULFONIC ACID: $C_6H_6SO_3$ (phenylsulfonic acid). Benzenesulfonic acid crystallizes as colorless plates from water. 14A020

PROPERTIES:

Molecular wt: 158.18; mp: 43-44, 65-66 (anhydrous); very soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Sulfonic acids are highly polar compounds. They are strong acids, being completely ionized in aqueous solutions. They may be fused with alkali to sulfonates which are hydrolyzed in acid to phenols.

Benzenesulfonic acid is decomposed by heat (100-175° C) to benzene and sulfuric acid.

The compound is decomposed by soil microflora in 16 days (ref. 3).

TOXIC PROPERTIES, HEALTH EFFECTS:

Benzenesulfonic acid is a strong acid. Contact of benzenesulfonic acid with the skin may result in irritation or burns. It is very irritating to skin, eyes, and mucous membranes (ref. 1).

LD_{50} (oral, rat): 890 mg/kg.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 890 = 4.0 \times 10^4$ μg/m^3
Water, Health: $15 \times 4.0 \times 10^4 = 6.0 \times 10^5$ μg/ℓ
Land, Health: $0.2 \times 6.0 \times 10^5 = 1.2 \times 10^5$ μg/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 890 = 95$ μg/m^3
$EPC_{AH3} = 0.081 \times 890 = 72$ μg/m^3
$EPC_{WH1} = 15 \times 72 = 1{,}080$ μg/ℓ
$EPC_{WH2} = 0.4 \times 890 = 356$ μg/ℓ
$EPC_{LH} = 0.2 \times 356 = 71$ μg/g

BENZENESULFONIC ACID

EMISSION LEVEL GOALS	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			4.0E4		72		
Water, μg/l (ppm Wt)			6.0E5		356		
Land, μg/g (ppm Wt)			1.2E5		70		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			72		
Water, μg/l (ppm Wt)			356		
Land, μg/g (ppm Wt)			70		

CATEGORY: 14A

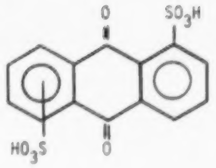
ANTHRAQUINONE-DISULFONIC ACIDS: 14A040

$C_{14}H_6O_2\ (SO_3H)_2$. A yellow crystalline solid.

9,10-ANTHRAQUINONE-1,5-DISULFONIC ACID. 14A041
9,10-ANTHRAQUINONE-1,6-DISULFONIC ACID. 14A042
9,10-ANTHRAQUINONE-1,7-DISULFONIC ACID. 14A043
9,10-ANTHRAQUINONE-1,8-DISULFONIC ACID. 14A044

WLN:

STRUCTURE:



PROPERTIES:

	mol. wt.	mp.
9,10-anthraquinone-1,5-disulfonic acid:	368.35	310-1 (decomposes)
9,10-anthraquinone-1,6-disulfonic acid:	368.35	215-7 (decomposes)
9,10-anthraquinone-1,7-disulfonic acid:	368.35	120 (decomposes)
9,10-anthraquinone-1,8-disulfonic acid:	368.35	293-4 (decomposes)

All are soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Sulfonic acids are used in the synthesis of dyes, elastomers, medicinals, pesticides, and plastics (ref. 2).

TOXIC PROPERTIES, HEALTH EFFECTS:

In general, sulfonic acids have not proved to be very hazardous. As a group, they are almost entirely free from serious systemic or cumulative effects. Even rings with amino or nitro groups are often relatively inert. The explanation probably derives from the rapid excretion in the urine, either unchanged or conjugated with glycine or glucuronic acid, and from a change in activity of functional groups. The presence of the acid in many cases seems to reduce or abolish the ability of the substance to penetrate through the skin, or cause the development of skin sensitivity (ref. 2).

LD_{50} (oral, rat): > 3,200 mg/kg for 1,8-anthraquinone disulfonic dipotassium salt,(ref. 2).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

* **MINIMUM ACUTE TOXICITY CONCENTRATIONS**:

Air, Health:	$45 \times 3{,}200 = 1.44 \times 10^5\ \mu g/m^3$	Air, Ecology:
Water, Health:	$15 \times 1.44 \times 10^5 = 2.16 \times 10^6\ \mu g/l$	Water, Ecology:
Land, Health:	$0.2 \times 2.16 \times 10^6 = 4.3 \times 10^5\ \mu g/g$	Land, Ecology:

* **ESTIMATED PERMISSIBLE CONCENTRATIONS**:

$EPC_{AC2} = 0.107 \times 3{,}200 = 342.4\ \mu g/m^3$

$EPC_{AC3} = 0.081 \times 3{,}200 = 260\ \mu g/m^3$

$EPC_{WH1} = 15 \times 260 = 3{,}900\ \mu g/l$

$EPC_{WH2} = 0.4 \times 3{,}200 = 1{,}280\ \mu g/l$

$EPC_{LH} = 0.2 \times 1{,}280 = 256\ \mu g/g$

* Based on LD_{50} for 1,8-Anthraquinone disulfonic dipotassium salt.

MULTIMEDIA ENVIRONMENTAL GOALS

14A040
ANTHRAQUINONE-DISULFONIC ACIDS

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.44E5		260		
Water, $\mu g/l$ (ppm Wt)			2.16E6		1,280		
Land, $\mu g/g$ (ppm Wt)			4.32E5		256		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			260		
Water, $\mu g/l$ (ppm Wt)			1,280		
Land, $\mu g/g$ (ppm Wt)			256		

REFERENCES: CATEGORY 14A

Sulfonic Acids, Sulfoxides - Sulfonic Acids

1. Windholz, M., Ed. The Merck Index: An Encyclopedia of Chemicals and Drugs, Ninth Edition. Merck & Co., Inc., Rahway, NJ (1976).

2. Fassett, D. W. Organic Acids, Anhydrides, Lactones, Acid Halides and Amides, Thioacids. Industrial Hygiene and Toxicology, Second Edition, Vol. 2. F. A. Patty, Ed., Interscience Publishers, New York, p. 1771-1837, 1962.

3. Verschueren, K. Handbook of Environmental Data on Organic Chemicals. Van Nostrand Rheinhold Company, NY (1977).

CATEGORY 14

SULFONIC ACIDS, SULFOXIDES

SUBCATEGORY: 14B - Sulfoxides

Summary of Subcategory

Total number of compounds in subcategory	1
number of parent compounds with subspecies	0
number of subspecies	0
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	1

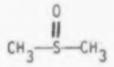
Consent Decree compounds included in subcategory: 0

CATEGORY: 14B

DIMETHYL SULFOXIDE: $(CH_3)_2SO$
(DMSO, methyl sulfoxide, sulfinylbis [methane]). 14B020
A colorless, odorless liquid with a slightly bitter taste
and sweet aftertaste; very hygroscopic.

WLN: OS1 & 1

STRUCTURE:



$$CH_3-\overset{\overset{O}{\|}}{S}-CH_3$$

PROPERTIES:

Molecular wt: 78.13; mp: 18.45; bp: 189^{760}; d: 1.1014^{20}_{4};
vap. d.: 2.71; vap. press: 0.42 mm at 20°C; soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Dimethyl sulfoxide is used as a solvent for gases, as antifreeze or hydraulic fluid when mixed with water, and as a paint and varnish remover (ref. 1). It can be formed by air-oxidation of dimethyl sulfide in the presence of nitrogen oxides (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

Skin contact with dimethyl sulfoxide results in primary irritation (ref. 1).

LD_{50} (intravenous, rat): 5,360 mg/kg (ref. 2).

Dimethyl sulfoxide has been reported to cause teratogenic effects in experimental animals (refs. 2,3).

The EPA/NIOSH ordering number based on teratogenicity is 4,314. The lowest dosage producing a teratogenic response is 50 mg/kg. The adjusted ordering number is 86.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$7 \times 10^4/86 = 814.0$ µg/m^3	Air, Ecology:	
Water, Health:	$15 \times 814.0 = 1.22 \times 10^4$ µg/l	Water, Ecology:	
Land, Health:	$0.2 \times 1.22 \times 10^4 = 2.4 \times 10^3$ µg/g	Land, Ecology:	

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 5,360 = 573.5$ µg/m^3

$EPC_{AH3} = 0.081 \times 5,360 = 434.2$ µg/m^3

$EPC_{WH1} = 15 \times 434.2 = 6,513$ µg/l

$EPC_{WH2} = 0.4 \times 5,360 = 2,144$ µg/l

$EPC_{LH} = 0.2 \times 2,144 = 429$ µg/g

$EPC_{AT} = 10^3/(6 \times 86) = 1.94$ µg/m^3

$EPC_{WT} = 15 \times 1.94 = 29.1$ µg/l

$EPC_{LT} = 0.2 \times 29.1 = 6$ µg/g

MULTIMEDIA ENVIRONMENTAL GOALS

X
14B020
DIMETHYL SULFOXIDE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			8.14E2		1.94		
Water, μg/l (ppm Wt)			1.22E4		29.1		
Land, μg/g (ppm Wt)			2.4E3		6		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			434.2		1.94
Water, μg/l (ppm Wt)			2,144		29.1
Land, μg/g (ppm Wt)			429		6

REFERENCES: CATEGORY 14B

Sulfonic Acids, Sulfoxides - Sulfoxides

1. Windholz, M., Ed. The Merck Index: An Encyclopedia of Chemicals and Drugs, Ninth Edition. Merck & Co., Inc., Rahway, NJ (1976).

2. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

3. Shepard, T. H. Catalog of Teratogenic Agents. Johns Hopkins University Press, Baltimore, MD (1973).

CATEGORY 15

BENZENE, SUBSTITUTED BENZENE HYDROCARBONS

SUBCATEGORY: 15A - Benzene and Monosubstituted Benzene Hydrocarbons

Summary of Subcategory

Total number of compounds in subcategory	10
number of parent compounds with subspecies	1
number of subspecies	3
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	1

Consent Decree compounds included in subcategory: 3

15A020	Benzene
15A040	Toluene
15A060	Ethyl benzene

CATEGORY: 15A

WLN: R

BENZENE: C_6H_6 (benzol, phenylhydride, phene).
A clear, colorless liquid. 15A020

STRUCTURE:

PROPERTIES:

Molecular wt: 78.11; mp: 5.5; bp: 80.1;
d: 0.87865^{20}_{4}; vap. press: 100 mm at 26.1° C; vap. d: 2.77;
solubility in water: 1,780 mg/ℓ at 25° (ref. 1); soluble in tissue lipids.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzene occurs in straight-run petroleum distillates and in coal-tar distillates. Rural background for benzene is reported as 0.1 ppbc (ref. 2). This is equivalent to 0.017 ppb or 0.054 μg/m^3. The odor recognition level is 10.5 to 210 mg/m^3 (ref. 3). Benzene participates to a very limited degree in photooxidation reactions (ref. 3). Benzene has been identified in at least one drinking water supply in the United States in concentrations as high as 10 μg/ℓ (ref. 4). There is a strong indication that plants may perform a major role in the degradation and synthesis of benzene in the environment (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

Benzene is an acute and chronic poison. It is absorbed through the skin, but most often poisoning occurs through inhalation. The rate of absorption of benzene through the skin has been reported to be 0.4 mg/cm^2/hr (ref. 5). It is estimated that 50 percent to 70 percent of benzene inhaled may be absorbed through the lungs (ref. 5). In acute poisoning cases, benzene acts as a narcotic. Chronic poisoning is characterized by damage to the blood-forming tissues and changes in body organs, including the lymph nodes (ref. 6). Inhalation of 210 ppm has resulted in blood disorders for exposed workers (ref. 7,8,9). Benzene can induce chromosomal aberrations in humans (ref. 6).

Benzene is indicated to be a carcinogen. The EPA/NIOSH ordering number is 7222. Inhalation of 2,100 mg/m^3 for 4 years has resulted in cancer in an exposed worker, and large doses of benzene painted repeatedly on the skin of mice have resulted in some incidence of skin carcinomas. Dosages associated with these tests are extremely high and are probably not indicative of the true carcinogenic potential of benzene. An epidemiological study conducted by NIOSH indicates that the incidence of leukemia in workers exposed to benzene is at least five times the expected incidence (ref. 6).

Benzene is toxic to aquatic life: 96 hour - TLm: 10-100 ppm (ref. 8).

Phytotoxicity: exposure for 35 minutes to 10 ppm of ozonated benzene produced red bordered spots on pinto beans (ref. 21). 10 ppm is equivalent to 30 mg/m^3. 24 hour exposure corrected concentration is 30,000 x 35/1440 = 729 μg/m^3 (0.24 ppm).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV: 30 mg/m^3 (10 ppm). ACGIH classified benzene as an Occupational Substance Suspected of Oncogenic Potential for workers. (Evidence linking benzene to leukemia was limited at the time the TLV was established.) Benzene appears on EPA Consent Decree List with an assigned priority of 1. Benzene was the subject of a 1974 NIOSH Criteria Document. The recommended 1974 standard was for 10 ppm as a time-weighted average with a ceiling of 25 ppm (Ref. 10). In February 1978, the Labor Department issued, to become effective in March, standards limiting worker exposure to benzene to 1 ppm as an 8-hour time-weighted average concentration, with a ceiling level of 5 ppm for any 15-minute period during the 8-hour day (ref. 6.) The standard also prohibits repeated or prolonged skin exposure to liquid benzene. The standard was based on conclusive evidence that exposure to benzene presents a leukemia hazard (ref. 6). 1 ppm is equivalent to 3 mg/m^3. The standard still has not been enacted due to cost.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 3.0×10^3 μg/m^3
Water, Health: $15 \times 3.0 \times 10^3 = 4.5 \times 10^4$ μg/ℓ
Land, Health: $0.2 \times 4.5 \times 10^4 = 9.0 \times 10^3$ μg/g

Air, Ecology: 729 μg/m^3 (0.2 ppm)
Water, Ecology: $100 \times 10 = 1.0 \times 10^3$ μg/ℓ
Land, Ecology: $0.2 \times 1.0 \times 10^3 = 200$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 30/420 = 71.4$ μg/m^3
$EPC_{AH1a} = 10/420 = 0.024$ ppm
$EPC_{WH1} = 15 \times 71.4 = 1{,}071$ μg/ℓ
$EPC_{WH2} = 13.8 \times 30 = 414$ μg/ℓ
$EPC_{LH} = 0.2 \times 414 = 83$ μg/g
$EPC_{AC1} = 10^3 \times 3/420 = 7.1$ μg/m^3
$EPC_{WC} = 15 \times 7.1 = 107$ μg/ℓ
$EPC_{LC} = 0.2 \times 107 = 21$ μg/g

$EPC_{AE} = 0.1 \times 729 = 72.9$ μg/m^3 (0.02 ppm)
$EPC_{WE1} = 50 \times 10 = 500$ μg/ℓ
$EPC_{LE} = 0.2 \times 500 = 100$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

X
15A020
BENZENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			3.0E3	7.29E2 (0.2)	7.1	73 (0.02)	0.054
Water, μg/l (ppm Wt)			4.5E4	1.0E3	107	500	10†
Land, μg/g (ppm Wt)			9.0E3	2.0E2	21	100	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			71.4 (0.024)	73 (0.02)	7.1
Water, μg/l (ppm Wt)			414	500	107
Land, μg/g (ppm Wt)			83	100	21

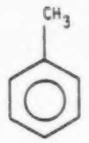
†Maximum level reported in public drinking water supplies.

CATEGORY: 15A

WLN: IR

TOLUENE: C_7H_8 (methylbenzene, toluol, phenylmethane).
A clear, colorless liquid; sweet, pungent, benzene-like odor. 15A040

STRUCTURE:



PROPERTIES:

Molecular wt: 92.13; mp: -96; bp: 110.6, $14.5^{14.5}$; d: 0.8669^{20}; insoluble in water; vap. press.: 36.7 mm at 30° C; vap. d: 3.14.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Toluene is a constituent of coal tar; it is generally associated with benzene and xylene. Rural concentration in air is reported as 3.0 to 18.2 ppbc (0.4 to 2.6 ppb, or 1.5 to 9.8 $\mu g/m^3$) (ref. 2).

Odor recognition level is reported as 1.03 to 140 $\mu g/m^3$ (0.27 to 37 ppb) (ref. 3) and the odor threshold level, 2.14 ppm (8 mg/m^3) (ref. 11). Toluene participates to a limited extent in photooxidation reactions (ref. 3).

Toluene has been found in samples of U.S. drinking water supplies in concentrations of 11 μg/ℓ (ref. 4).

TOXIC PROPERTIES, HEALTH EFFECTS:

Acute poisoning may result from exposure to high concentrations of toluene; a narcotic effect is produced. Human death has resulted from exposure to 10,000 ppm (ref. 7). Toluene is more acutely toxic than benzene; however, severe blood disorders of the type associated with benzene are not reported. Inhalation of 100 ppm has resulted in psychological effects and 200 ppm has affected the central nervous system in humans (ref. 8). Irritative effects to eyes, mucous membranes, and the upper respiratory tract have resulted from exposure to 200 to 500 ppm (ref. 12). Toluene may be absorbed through the skin as well as by inhalation (ref. 12), although the inhalation route is far more important. There is evidence to indicate that at equilibrium, the average toluene concentration per liter of blood is 2.4 mg for each 100 ppm toluene in the environmental air (ref. 13). The biological half-life for toluene is reported to be 0.083 days (ref. 14).

LD_{50} (oral, rat): 5,000 mg/kg. LC_{Lo} (inhalation, rat): 4,000 ppm for 4 hours.

Aquatic toxicity: TLm 96: 100-10 ppm (ref. 8). Concentrations of 0.25 mg/ℓ can cause tainting of fish flesh (ref. 15).

Phytotoxicity: exposure for 35 minutes to 50 ppm of ozonated toluene produced a bronze color on pinto beans (ref. 21). 50 ppm is equivalent to 188 mg/m^3. 24 hr. exposure corrected concentration is $188 \times 10^3 \times .35/1440 =$ 4,570 $\mu g/m^3$ (1.2 ppm).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 375 mg/m^3 (100 ppm). Toluene is on EPA's Consent Decree Priority III List.

Toluene is the subject of a NIOSH Criteria Document. The NIOSH recommendation for occupational exposure to toluene is 100 ppm as an 8-hour per work day time-weighted average. A ceiling value of 200 ppm is recommended (ref. 12).

Toluene is on the First Priority Chemicals List of Chemical Industry Institute of Toxicology.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 3.75×10^5 $\mu g/m^3$ (100 ppm)
Water, Health: $15 \times 3.75 \times 10^5 = 5.6 \times 10^6$ μg/ℓ
Land, Health: $0.2 \times 5.6 \times 10^6 = 1.1 \times 10^6$ μg/g

Air, Ecology: 4.57×10^3 $\mu g/m^3$ (1.2 ppm)
Water, Ecology: $100 \times 10 = 1 \times 10^3$ μg/ℓ
Land, Ecology: $0.2 \times 1 \times 10^3 = 200$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 375/420 = 893$ $\mu g/m^3$
$EPC_{AH1a} = 100/420 = 0.24$ppm
$EPC_{WH1} = 15 \times 893 = 13,400$ μg/ℓ
$EPC_{WH2} = 13.8 \times 375 = 5,175$ μg/ℓ
$EPC_{LH} = 0.2 \times 5,175 = 1,035$ μg/g

$EPC_{AE} = 0.1 \times 4,570 = 457$ $\mu g/m^3$ (0.12 ppm)

$EPC_{WE1} = 50 \times 10 = 500$ μg/ℓ
$EPC_{WE2} = 250$ μg/ℓ (to prevent tainting)
$EPC_{LE} = 0.2 \times 250 = 50$ μg/g

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)			3.75E5 (100)	4.57E3 (1.2)	893 (0.24)	457 (0.12)	1.5 to 9.8
Water, μg/l (ppm Wt)			5.6E6	1.0E3	5,175	250	11†
Land, μg/g (ppm Wt)			1.1E6	2.0E2	1,000	50	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)			893 (0.24)	457 (0.12)	
Water, μg/l (ppm Wt)			5,175	250	
Land, μg/g (ppm Wt)			1,000	50	

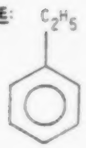
†Drinking water supplies.

CATEGORY: 15A

WLN: 2R

ETHYL BENZENE: C_8H_{10} (ethyl benzol, phenylethane).
A colorless liquid; aromatic odor. 15A060

STRUCTURE:



PROPERTIES:

Molecular wt: 106.16; fp: -94.9; bp: 136.2; d: 0.8669^{25}_{25};
vap. press.: 10 mm at 25.9°; vap. d: 3.66; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Rural concentration in air is reported as 0.5 to 1.6 ppbc (ref. 2). This is equivalent to 0.06-0.20 ppb or 0.3-0.87 $\mu g/m^3$. Urban concentrations as high as 111 ppbc (13.9 ppb, or 60 $\mu g/m^3$) have been reported (ref. 2).

TOXIC PROPERTIES, HEALTH EFFECTS:

Ethyl benzene is an irritant to mucous membranes, skin, and eyes; and a narcotic in high concentrations. It is the most severe skin irritant of the benzene series. A concentration of 200 ppm causes eye irritation and gives warning of dangerous concentrations (refs. 7, 13). A concentration of 100 ppm for 8 hours caused irritative effects in a human (ref. 8). It is absorbed through the skin as well as through the lungs. No chronic effects of exposure are reported.

LD_{50} (oral, rat): 3,500 mg/kg.
LC_{Lo} (inhalation, rat): 4,000 ppm for 4 hours.
Aquatic toxicity: TLm 96: 100-10 ppm (ref. 8).
Concentrations of: <0.25 mg/ℓ can cause tainting of fish flesh (ref. 15).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 435 mg/m^3 (100 ppm).
On EPA's Consent Decree Priority III List.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 4.35×10^5 $\mu g/m^3$ (100 ppm)
Water, Health: $15 \times 4.35 \times 10^5 = 6.5 \times 10^6$ $\mu g/\ell$
Land, Health: $0.2 \times 6.5 \times 10^6 = 1.3 \times 10^6$ $\mu g/g$

Air, Ecology:
Water, Ecology: $100 \times 10 = 1.0 \times 10^3$ $\mu g/\ell$
Land, Ecology: $0.2 \times 1.0 \times 10^3 = 200$ $\mu g/g$

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 435/420 = 1{,}040\ \mu g/m^3$
$EPC_{AH1a} = 100/420 = 0.24$ ppm
$EPC_{WH1} = 15 \times 1{,}040 = 15{,}600\ \mu g/\ell$
$EPC_{WH2} = 13.8 \times 435 = 6{,}000\ \mu g/\ell$
$EPC_{LH} = 0.2 \times 6{,}000 = 1{,}200\ \mu g/g$

$EPC_{WE1} = 50 \times 10 = 500\ \mu g/\ell$
$EPC_{WE2} = 250\ \mu g/\ell$ (to prevent tainting)
$EPC_{LE} = 0.2 \times 250 = 50\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

15A060
ETHYL BENZENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)			4.35E5 (100)		1,040 (0.24)		0.3 to 0.87
Water, μg/l (ppm Wt)			6.5E6	1.0E3	6,000	250	
Land, μg/g (ppm Wt)			1.3E6	2.0E2	1,200	50	

*To be multiplied by dilution factor

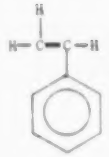
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)			1,040 (0.24)		
Water, μg/l (ppm Wt)			6,000	250	
Land, μg/g (ppm Wt)			1,200	50	

CATEGORY: 15A

WLN: 1U1R

STYRENE: C_8H_{12} (phenylethylene, ethenylbenezene, vinyl benzene, styrolene). 15A080
A colorless, oily liquid with a penetrating aromatic odor.

STRUCTURE:



PROPERTIES:

Molecular wt: 104.16; mp: -30.63; bp: 145.2^{760};
d: 0.9060^{20}_{4}; vap. d: 3.6; sparing soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Styrene is formed from ethylbenzene by dehydrogenation (ref. 16). It is used industrially as a starting material for the production of various polymers (ref. 17). It also occurs naturally in the sap of styraceous trees (ref. 13).

Odor threshold in air for styrene is 0.1 ppm (inhibited) and 0.047 (uninhibited)(ref. 11). Urban atmosphere concentration has been reported as 76 ppbc, or 40.4 μg/m^3(ref. 2). Styrene has also been reported in samples taken from drinking water, with the highest reported concentration of <1.0 μg/l (ref. 4).

TOXIC PROPERTIES, HEALTH EFFECTS:

Exposure to styrene may produce severe human eye irritation and injury (ref. 9). It may also produce respiratory tract irritation, dermatitis, and anxiety (ref. 18). The vapor at concentrations of 200 to 400 ppm has a transient irritating effect on the eyes (ref. 13). Human death has resulted from exposure to 10,000 ppm for 30 minutes (ref. 8). Human exposure to 376 ppm has produced central nervous system effects (ref. 8). No chronic toxicity has been reported associated with exposure to styrene (ref. 17).

Absorption of styrene is mainly through the respiratory tract. In both animals and man, styrene is metabolized to benzoic acid, conjugated with glycine, and excreted in the urine as hippuric acid. As long as styrene is present in the circulating blood, some of it is excreted in the exhaled air (ref. 13).

LD_{50} (oral, rat): 5,000 mg/kg (ref. 8).

Aquatic toxicity: TLm 96: 100-10 ppm (ref. 8).

A concentration of 0.25 mg/l in water is reported to cause the tainting of fish flesh (ref. 15).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 420 mg/m^3 (100 ppm).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	10^3 x 420 = 4.2 x 10^5 μg/m^3 (100 ppm)	Air Ecology:	
Water, Health:	15 x 4.2 x 10^5 = 6.3 x 10^6 μg/l	Water, Ecology:	100 x 10 = 1,000 μg/l
Land, Health:	0.2 x 6.3 x 10^6 = 1.26 x 10^6 μg/g	Land, Ecology:	0.2 x 1,000 = 200 μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

EPC_{AH1} = 10^3 x 420/420 = 1,000 μg/m^3	
EPC_{AH1a} = 100/420 = 0.24 ppm	
EPC_{WH1} = 15 x 1,000 = 1.5 x 10^4 μg/l	EPC_{WE1} = 50 x 10 = 500 μg/l
EPC_{WH2} = 13.8 x 420 = 5,800 μg/l	EPC_{WE2} = 250 μg/l (to prevent tainting)
EPC_{LH} = 0.2 x 5,800 = 1,160 μg/g	EPC_{LE} = 0.2 x 250 = 50 μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

15A080 STYRENE

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			4.2E5 (100)		1,000 (0.24)		40.4†
Water, μg/l (ppm Wt)			6.3E6	1.0E3	5,800	250	<1.0‡
Land, μg/g (ppm Wt)			1.26E6	2.0E2	1,160	50	

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			1,000 (0.24)		
Water, μg/l (ppm Wt)			5,800	250	
Land, μg/g (ppm Wt)			1,160	50	

†Urban atmosphere.

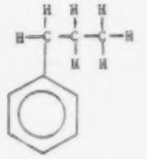
‡Maximum level reported in public drinking water supplies.

CATEGORY: 15A

PROPYL BENZENE: C_9H_{12} (1-phenyl propane).
A clear liquid. 15A100

WLN: 3R

STRUCTURE:



PROPERTIES:

Molecular wt: 120.20; mp: -99.5; bp: 159.2^{760}; d: 0.8620^{20}_{4};
vap. press: 10 mm at 43.4°; vap.d· 4.14; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Rural background atmosphere concentration is reported as 0.1 to 1.1 ppbc (ref. 2). This is equivalent to 0.05 to 0.6 $\mu g/m^3$. It has also been reported in public drinking water supplies, with the highest reported concentration at <5.0 $\mu g/l$ (ref. 4).

Propyl benzene is used in textile dyeing and printing, and as a solvent for cellulose acetate (ref. 16). It occurs in petroleum distillates and in coal tar derivatives.

TOXIC PROPERTIES, HEALTH EFFECTS:

Acute toxicity of propyl benzene is expected to be similar to that of ethylbenzene and isopropyl benzene.

LD_{Lo} (oral, rat): 4,830 mg/kg

LD_{50} (oral, rat): 3,500 mg/kg for ethylbenzene, and 1,400 mg/kg for isopropyl benzene (ref. 8).

LD_{Lo} (inhalation, mouse): 4,100 ppm, 2,000 ppm for isopropyl benzene (ref. 8).

Aquatic toxicity: Likely to be similar to that of other alkyl benzene compounds.

TLm 96: 100-10 ppm for isopropyl benzene (ref. 8).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV for isopropyl benzene is 250 mg/m^3 (50 ppm).

* MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $10^3 \times 250 = 2.5 \times 10^5\ \mu g/m^3$ (50 ppm)
Water, Health: $15 \times 2.5 \times 10^5 = 3.75 \times 10^6\ \mu g/l$
Land, Health: $0.2 \times 3.75 \times 10^6 = 7.5 \times 10^5\ \mu g/g$

Air, Ecology:
Water, Ecology: $100 \times 10 = 1{,}000\ \mu g/l$
Land, Ecology: $0.2 \times 1{,}000 = 200\ \mu g/g$

* ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 250/420 = 595\ \mu g/m^3$
$EPC_{AH1a} = 50/420 = 0.12$ ppm
$EPC_{WH1} = 15 \times 595 = 8{,}930\ \mu g/l$
$EPC_{WH2} = 13.8 \times 250 = 3{,}450\ \mu g/l$
$EPC_{LH} = 0.2 \times 3{,}450 = 690\ \mu g/g$

$EPC_{WE1} = 50 \times 10 = 500\ \mu g/l$
$EPC_{WE2} = 250\ \mu g/l$ (to prevent tainting)
$EPC_{LE} = 0.2 \times <250 = 50\ \mu g/g$

*Based on data for isopropyl benzene.

MULTIMEDIA ENVIRONMENTAL GOALS

15A100
PROPYL BENZENE

EMISSION LEVEL GOALS †

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.5E5		595 (0.12)		0.05 to 0.6
Water, $\mu g/l$ (ppm Wt)			3.75E6	1.0E3	3,450	250	< 5.0‡
Land, $\mu g/g$ (ppm Wt)			7.5E5	2.0E2	690	50	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS†

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Basedon Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			595 (0.12)		
Water, $\mu g/l$ (ppm Wt)			3,450	250	
Land, $\mu g/g$ (ppm Wt)			690	50	

†Based on data for isopropyl benzene.

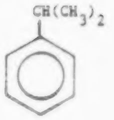
‡Public drinking water supplis.

CATEGORY: 15A

ISOPROPYL BENZENE: C_9H_{12} [(1-methyl ethyl) benzene, isopropyl benzol, 2-phenylpropane, cumene].
A colorless liquid with a sharp aromatic odor. 15A120

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 120.20; mp: -96; bp: 152.4^{760}; d: 0.8618$^{20}_{4}$;
vap. d: 4.1; vap. press: 10 mm at 38.3°; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Isopropyl benzene has been reported in urban atmosphere in concentrations of 76 ppbc. This is equivalent to 41 μg/m^3 (ref. 2). It has been reported in samples taken from well water, river water, and finished drinking water (ref. 19). The highest concentration reported in drinking water is 0.01 μg/l (ref. 4).

Isopropyl benzene is found in American petroleum (ref. 16). It is used for synthesis in the chemical industry and as a thinner for paints and enamels (ref. 13).

Methods for determining vapor in air are similar to those used for xylene (ref. 13).

TOXIC PROPERTIES, HEALTH EFFECTS:

Isopropyl benzene may produce conjunctivitis, dermatitis, and irritation of the respiratory tract. It is a central nervous system depressant and may also produce spleen and liver changes (ref. 13).

Small quantities of isopropyl benzene absorbed in the blood are exhaled unchanged, but the major portion is metabolized in the liver and excreted in the urine as conjugated alcohols or acids (ref. 7). There is no evidence of damage to blood-forming tissues or other chronic effects from repeated exposure to isopropyl benzene (ref. 13).

LD_{50} (oral, rat): 1,400 mg/kg (ref. 8)
LC_{50} (inhalation, rat): 8,000 ppm/4 hours, LC_{Lo} (inhalation, mouse): 2,000 ppm (ref. 8).
Aquatic toxicity: TLm 96: 100-10 ppm (ref. 8)

A concentration of isopropyl benzene of <0.25 mg/l can cause tainting of the flesh of fish and other aquatic organisms (ref. 15).

Phytotoxicity: exposure for 35 minutes to 10 ppm of ozonated isopropyl benzene produced unspecified effects in pinto beans (ref. 21). 10 ppm is equivalent to 50 mg/m^3. 24-hour exposure corrected concentration is 50,000 x 35/1440 = 1,215 μg/m^3 (0.25 ppm).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 250 mg/m^3 (50 ppm).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $10^3 \times 250 = 2.5 \times 10^5$ μg/m^3 (50 ppm)
Water, Health: $15 \times 2.5 \times 10^5 = 3.75 \times 10^6$ μg/l
Land, Health: $0.2 \times 3.75 \times 10^6 = 7.5 \times 10^5$ μg/g

Air, Ecology: 1,215 μg/m^3 (0.25 ppm)
Water, Ecology: $100 \times 10 = 1{,}000$ μg/l
Land, Ecology: $0.2 \times 1{,}000 = 200$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 250/420 = 595$ μg/m^3
$EPC_{AH1a} = 50/420 = 0.12$ ppm
$EPC_{WH1} = 15 \times 595 = 8{,}930$ μg/l
$EPC_{WH2} = 13.8 \times 250 = 3{,}450$ μg/l
$EPC_{LH} = 0.2 \times 3{,}450 = 690$ μg/g

$EPC_{AE} = 0.1 \times 1{,}215 = 121$ μg/m^3 (0.025 ppm)
$EPC_{WE1} = 50 \times 10 = 500$ μg/l
$EPC_{WE2} =$ 250 μg/l (to prevent tainting)
$EPC_{LE} = 0.2 \times 250 = 50$ μg/g

15A120
ISOPROPYL BENZENE

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)			2.5E5 (50)	1.2E3 (0.25)	595.2 (0.12)	121 (0.025)	41
Water, μg/l (ppm Wt)			3.75E6	1.0E3	3,450	250	0.01⁺
Land, μg/g (ppm Wt)			7.5E5	2.0E2	690	50	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)			595 (0.12)	121 (0.025)	
Water, μg/l (ppm Wt)			3,450	250	
Land, μg/g (ppm Wt)			690	50	

⁺Public drinking water supplies.

CATEGORY: 15A

WLN:

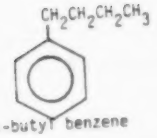
BUTYL BENZENES: $C_{10}H_{14}$. 15A140

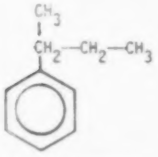
n-BUTYL BENZENE: (1-phenyl butane). Colorless liquid. 15A141

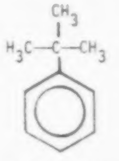
sec-BUTYL BENZENE: (2-phenyl butane, 1-methylpropyl benzene). Colorless liquid. 15A142

tert-BUTYL BENZENE: ((1,1-Dimethylethyl)benzene, 2-methyl-2-phenyl propane, trimethylphenyl methane, pseudobutyl benzene). Colorless liquid. 15A143

STRUCTURE:


n-butyl benzene


sec-butyl benzene


tert-butyl benzene

PROPERTIES:

	molecular wt.	m.p.	b.p.	d.	vap. press	vap.d.	solubility in water
n-butyl benzene	134.22	-88	183^{760}	0.8601_4^{20}	1 mm at 22.7°	4.6	insoluble
sec-butyl benzene	134.22	-75	173^{760}	0.8621_4^{20}	1 mm at 18.6°	4.62	insoluble
tert-butyl benzene	134.22	-57.85	169^{760}	0.8665_4^{20}	1 mm at 13.0°	4.62	insoluble

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Butyl benzene has been reported in samples taken from river water and from finished drinking water (ref. 19). sec-Butyl benzene is prepared from benzene and n-butyl chloride in the presence of $AlCl_3$ (ref. 16). tert-Butyl benzene can be formed from isobutyl alcohol and benzene by treatment with fuming sulfuric acid (ref. 16). sec-Butyl benzene is used as a solvent and in organic synthesis (ref. 16).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxic effects of butyl benzenes are expected to be similar to those of the other alkyl benzene compounds.

n-Butyl benzene: LD_{Lo} (oral, rat): 5,000 mg/kg (ref. 8).

sec-Butyl benzene: LD_{50} (oral, rat): 2,240 mg/kg (ref. 8).

tert-Butyl benzene: LD_{Lo} (oral, rat): 5,000 mg/kg (ref. 8).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

* **MINIMUM ACUTE TOXICITY CONCENTRATIONS:**

Air, Health: $45 \times 2,240 = 1.01 \times 10^5$ μg/m³

Water, Health: $15 \times 1.01 \times 10^5 = 1.52 \times 10^6$ μg/l

Land, Health: $0.2 \times 1.52 \times 10^6 = 3.04 \times 10^5$ μg/g

Air, Ecology:

Water, Ecology:

Land, Ecology:

* **ESTIMATED PERMISSIBLE CONCENTRATIONS:**

$EPC_{AH2} = 0.107 \times 2,240 = 240$ μg/m³

$EPC_{AH3} = 0.081 \times 2,240 = 181$ μg/m³

$EPC_{WH1} = 15 \times 181 = 2,715$ μg/l

$EPC_{WH2} = 0.4 \times 2,240 = 896$ μg/l

$EPC_{LH} = 0.2 \times 896 = 1,800$ μg/g

*Calculated from LD_{50} for sec-butyl benzene.

15A140
BUTYL BENZENES

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.0E5		181		
Water, $\mu g/l$ (ppm Wt)			1.5E6		896		
Land, $\mu g/g$ (ppm Wt)			3.0E5		1,800		

*To be multiplied by dilution factor

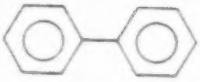
	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			181		
Water, $\mu g/l$ (ppm Wt)			896		
Land, $\mu g/g$ (ppm Wt)			1,800		

CATEGORY: 15A

WLN: RR

BIPHENYL: $C_{12}H_{10}$ (bibenzene, diphenyl, phenylbenzene).
White or colorless scales; pleasant odor. 15A160

STRUCTURE:



PROPERTIES:

Molecular wt: 154.2; mp: 71; bp: 255.9; d: 0.8660^{20},
vap.d: 5.31; vap. press: 1 mm at 70.6°; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Biphenyl is produced by thermal dehydrogenation of benzene (ref. 13). It is used as a heat transfer agent and in organic synthesis (ref. 16). It is one of the most thermally stable of known organic compounds (ref. 13).

Biphenyl has been reported in samples taken from finished drinking water (ref. 19).

TOXIC PROPERTIES, HEALTH EFFECTS:

Reported effects resulting from exposure to biphenyl include irritation and injury to respiratory passages; no chronic effects are documented (ref. 7). Exposure by inhalation to 4,400 $\mu g/m^3$ caused irritative effects in a human (ref. 8).

LD_{50} (oral, rat): 3,280 mg/kg.

Aquatic toxicity: Bioconcentration factor (calculated): 436 (ref. 20).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 1 mg/m^3 (0.2 ppm).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 1.0×10^3 $\mu g/m^3$ (0.2 ppm)	Air, Ecology:
Water, Health: $15 \times 1.0 \times 10^3 = 1.5 \times 10^4$ $\mu g/l$	Water, Ecology:
Land, Health: $0.2 \times 1.5 \times 10^4 = 3.0 \times 10^3$ $\mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 1/420 = 2.4$ $\mu g/m^3$
$EPC_{AH1a} = 0.2/420 = 0.0005$ ppm
$EPC_{WH1} = 15 \times 2.4 = 36$ $\mu g/l$
$EPC_{WH2} = 13.8 \times 1 = 13.8$ $\mu g/l$
$EPC_{LH} = 0.2 \times 13.8 = 3$ $\mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

15A160
BIPHENYL

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			1.0E3 (0.2)		2.4 (0.0005)		
Water, μg/l (ppm Wt)			1.5E4		13.8		
Land, μg/g (ppm Wt)			3.0E3		3		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			2.4 (0.0005)		
Water, μg/l (ppm Wt)			14		
Land, μg/g (ppm Wt)			3		

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Benzene, Substituted Benzene Hydrocarbons -
Benzene and Monosubstituted Benzene Hydrocarbons

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CATEGORY 15

BENZENE, SUBSTITUTED BENZENE HYDROCARBONS

SUBCATEGORY: 15B - Disubstituted and Polysubstituted Benzene Hydrocarbons

Summary of Subcategory

Total number of compounds in subcategory	23
number of parent compounds with subspecies	6
number of subspecies	20
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

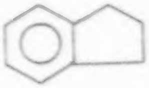
Consent Decree compounds included in subcategory: None

CATEGORY: 15B

WLN: L56T&J

INDAN: C_9H_{10} (hydrindene, 2,3-dihydroindene).
A colorless liquid. 15B020

STRUCTURE:



PROPERTIES:

Molecular wt: 118.19; mp: -51.4; bp: 176; d: 0.964;
insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Indan is present in coal tar. In processes such as coal gasification, indan will likely be converted to indene.

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{Lo} (oral, rat): 5,000 mg/kg.

Indan may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 2).

Indan is not included in the compounds tested thus far for carcinogenic activity (ref. 3).

Aquatic toxicity: 96-hr LC_{50} (fathead minnow): 14 mg/l (ref. 16).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 5,000 = 2.25 \times 10^5$ µg/m³
Water, Health: $15 \times 2.25 \times 10^5 = 3.4 \times 10^6$ µg/l
Land, Health: $0.2 \times 3.4 \times 10^6 = 6.8 \times 10^5$ µg/g

Air, Ecology:
Water, Ecology: $100 \times 14 = 1,400$ µg/l
Land, Ecology: $0.2 \times 1,400 = 280$ µg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 5,000 = 535$ µg/m³
$EPC_{AH1} = 0.081 \times 5,000 = 405$ µg/m³
$EPC_{WH1} = 15 \times 4.05 \times 10^2 = 6,000$ µg/l
$EPC_{WH2} = 0.4 \times 5,000 = 2,000$ µg/l
$EPC_{LH} = 0.2 \times 2,000 = 400$ µg/g

$EPC_{WE} = 50 \times 14 = 700$ µg/l
$EPC_{LE} = 0.2 \times 700 = 140$ µg/g

MULTIMEDIA ENVIRONMENTAL GOALS

15B020
INDAN

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, µg/m^3 (ppm Vol)			2.25E5		405		
Water, µg/l (ppm Wt)			3.4E6	1.4E3	2,000	700	
Land, µg/g (ppm Wt)			6.8E5	2.8E2	400	140	

*To be multiplied by dilution factor

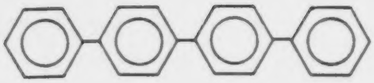
AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, µg/m^3 (ppm Vol)			405		
Water, µg/l (ppm Wt)			2,000	700	
Land, µg/g (ppm Wt)			400	140	

CATEGORY: 15B
4,4'-DIPHENYLBIPHENYL: $C_{24}H_{20}$ (p,p'-quaterphenyl, tetraphenyl). 15B060

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 306.41; mp: 320; bp: 428^{18}; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for 4-4' diphenylbiphenyl are not available at this time. However, toxicological characteristics of 4,4' diphenylbiphenyl are likely to be similar to those of biphenyl and terphenyl because of its chemical structure similarity. The data for these substances are shown below.

	TLV		LD_{50} (oral, rat)
Chemical	(mg/m^3)	(ppm)	(mg/kg)
biphenyl	1	0.2	3,280
terphenyl	9.4	1	500 (p-terphenyl)

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV: 1 mg/m^3 (0.2 ppm) for biphenyl.

***MINIMUM ACUTE TOXICITY CONCENTRATIONS:**

Air, Health: 1.99×10^3 µg/m^3 (0.2 ppm)	Air, Ecology:
Water, Health: $15 \times 1.99 \times 10^3 = 2.99 \times 10^4$ µg/l	Water, Ecology:
Land, Health: $0.2 \times 2.99 \times 10^4 = 5.98 \times 10^3$ µg/g	Land, Ecology:

***ESTIMATED PERMISSIBLE CONCENTRATIONS:**

$EPC_{AHi} = 10^3 \times 1.99/420 = 4.74$ µg/m^3

$EPC_{AH1a} = 0.2/420 = 4.8 \times 10^{-4}$ ppm

$EPC_{WH1} = 15 \times 4.74 = 71.1$ µg/l

$EPC_{WH2} = 13.8 \times 1.99 = 27.5$ µg/l

$EPC_{LH} = 0.2 \times 27.5 = 5.5$ µg/g

---

*Based on TLV for biphenyl; molecular wt ratio = $\frac{306.4\ (4,4'\text{-diphenylbiphenyl})}{154.2\ (\text{biphenyl})} = 1.99$

MULTIMEDIA ENVIRONMENTAL GOALS

15B060
4,4′-DIPHENYLBIPHENYL

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			2.0E3 (0.2)		5 (4.8×10^{-4})		
Water, μg/l (ppm Wt)			3.0E4		28		
Land, μg/g (ppm Wt)			6.0E3		6		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			5 (4.8×10^{-4})		
Water, μg/l (ppm Wt)			28		
Land, μg/g (ppm Wt)			6		

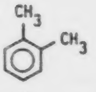
CATEGORY: 15B

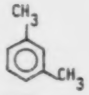
WLN: 1RB; 1RC; 1RD

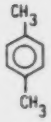
XYLENES: C_8H_{10} (dimethylbenzene, xylol). 15B080

A mobile, flammable liquid.
o-XYLENE: colorless liquid. 15B081
m-XYLENE: colorless liquid. 15B082
p-XYLENE: colorless plates or prisms at low temperature. 15B083

STRUCTURE:


ortho-


meta-


para-

PROPERTIES:

	Mol. wt	d_4^{20}	mp	bp	Water Solubility	Vap. d	Vap. press
m-xylene	106.2	0.864	-47.4	139.3	insoluble	3.66	10 mm at 28.3°
o-xylene	106.2	0.880	-25	144	"	3.66	10 mm at 32.1°
p-xylene	106.2	0.861	13-14	137-138	"	3.66	10 mm at 27.3°

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Xylenes include meta, ortho, and para structures. The meta isomer predominates in mixtures. The odor threshold in air for p-xylene is 0.47 ppm (2 mg/m^3) (ref. 4). Rural background concentrations are reported as follows (ref. 5):

	Rural Concentration
m-xylene	1.1-9.7 ppbc (0.14-1.2 ppb; 0.6-5.2 μg/m^3)
o-xylene	3.4-7.0 ppbc (0.43-0.88 ppb; 1.9-3.8 μg/m^3)
p-xylene	0.5-1.6 ppbc (0.06-0.2 ppb; 0.3-0.9 μg/m^3)

All three isomers have been found in samples of U.S. drinking water supplies in concentrations less than 5 μg/ℓ (ref. 6). The xylenes are obtained from coal tar. They are commonly used as solvents and as a raw material in synthesis of a variety of chemicals (ref. 8).

TOXIC PROPERTIES, HEALTH EFFECTS:

Xylenes are absorbed through skin as well as by inhalation (ref. 7). They may be narcotic in high concentrations. Chronic toxicity is not well known, but xylenes are considered less toxic than benzene (ref. 8). Effects of exposure to xylenes may be similar to effects from toluene but with a higher degree of toxicity (ref. 9). Concentration of 200 ppm is irritating to eyes, nose, and throat (refs. 9, 10). Since occurrence of xylenes is generally associated with benzene, the specific toxic potential of xylenes is difficult to isolate.

	LD_{50} (oral, rat)	LC_{Lo} (inhalation, rat)	LC_{Lo} (inhalation, mouse)	Aquatic toxicity
m-xylene	5,000 mg/kg	8,000 ppm/4 hours	--	--
o-xylene	5,000 mg/kg	--	6,920 ppm	TLm96: 100-10 ppm
p-xylene	5,000 mg/kg	--	3,460 ppm	TLm96: 100-10 ppm
xylene (mixture)	4,300 mg/kg	6,700 ppm/4 hours	--	TLm96: 100-10 ppm

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 435 mg/m^3 (100 ppm).

Xylene is the subject of a NIOSH criteria document. The NIOSH recommendation for occupational exposure to xylene is 100 ppm as a 10-hour-workday, time-weighted average. A ceiling of 200 ppm is recommended. (Xylene as used in the document refers to any one of a combination of the isomers of xylene) (ref. 11).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 4.35×10^5 μg/m^3 (100 ppm)
Water, Health: $15 \times 4.35 \times 10^5 = 6.5 \times 10^6$ μg/ℓ
Land, Health: $0.2 \times 6.5 \times 10^6 = 1.3 \times 10^6$ μg/g

Air, Ecology:
Water, Ecology: $100 \times 10 = 1.0 \times 10^3$ μg/ℓ
Land, Ecology: $0.2 \times 1.0 \times 10^3 = 200$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 435/420 = 1{,}040$ μg/m^3
$EPC_{AH1a} = 100/420 = 0.24$ ppm
$EPC_{WH1} = 15 \times 1{,}040 = 15{,}600$ μg/ℓ
$EPC_{WH2} = 13.8 \times 435 = 6{,}000$ μg/ℓ
$EPC_{LH} = 0.2 \times 6{,}000 = 1{,}200$ μg/g

$EPC_{WE1} = 50 \times 10 = 500$ μg/ℓ
$EPC_{LE} = 0.2 \times 500 = 100$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

15B080
XYLENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)			4.35E5 (100)		1,040 (0.24)		0.3 to 5.2
Water, μg/l (ppm Wt)			6.5E6	1.0E3	6,000	500	< 5⁺
Land, μg/g (ppm Wt)			1.3E6	2.0E2	1,200	100	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)			1,040 (0.24)		
Water, μg/l (ppm Wt)			6,000	500	
Land, μg/g (ppm Wt)			1,200	100	

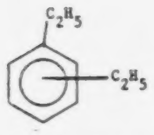
⁺Drinking water supplies.

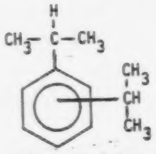
CATEGORY: 15B

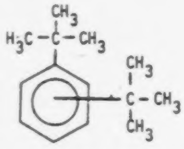
WLN: 2R X2/

DIALKYL BENZENES, (mw: 134-191) 15B100
o-DIETHYL BENZENE: $(C_2H_5)_2C_6H_4$. A colorless liquid. 15B101
m-DIETHYL BENZENE: $(C_2H_5)_2C_6H_4$. A colorless liquid. 15B102
p-DIETHYL BENZENE: $(C_2H_5)_2C_6H_4$. A colorless liquid. 15B103
o-DIISOPROPYL BENZENE: $(C_3H_7)_2C_6H_4$. A colorless liquid. 15B104
m-DIISOPROPYL BENZENE: $(C_3H_7)_2C_6H_4$. A colorless liquid. 15B105
1,4-DI-tert-BUTYL BENZENE: $(C_4H_9)_2C_6H_4$. A solid. 15B106

STRUCTURE:


diethyl benzene


diisopropyl benzene


di-tert-butyl benzene

PROPERTIES:

	mol.wt.	mp:	bp.	d	vap. d.	vap. p.	water solubility
o-diethyl benzene	134.22	-31.4	183.5	0.8800	4.62	1 mm at 20.7°	insoluble
m-diethyl benzene	134.22	-43.2	183.8	0.8602	(MIXTURE)	(MIXTURE)	insoluble
p-diethyl benzene	134.22	-83.9	181.1	0.8620			insoluble
o-diisopropyl benzene	162.28		210	0.858			insoluble
m-diisopropyl benzene	162.28	-105	202	0.860			insoluble
1,4-di-tert-butyl benzene	190.33	80-1	237				insoluble

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Diethylbenzene has been reported in samples taken from public drinking water supplies with the highest concentration reported to be 1.0 μg/l (ref. 6). It has also been found in well water and ground water (refs. 6, 12).

TOXIC PROPERTIES, HEALTH EFFECTS:

Chemical	LD_{Lo} (oral, rat)	Aquatic toxicity
o-diethyl benzene	5,000 mg/kg	
m-diethyl benzene	5,000 mg/kg	
diethyl benzene (MIXTURE)	5,000 mg/kg	TLm 96: 100-10 ppm.
o-diisopropyl benzene	5,000 mg/kg	

These compounds are probably similar to xylenes in their toxicity. There is no reason to believe that dialkyl benzenes (molecular weight 134-191) are more toxic than xylenes.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV for xylenes is 435 mg/m^3 (100 ppm).

* **MINIMUM ACUTE TOXICITY CONCENTRATIONS:**

Air, Health: 4.35×10^5 μg/m^3 (100 ppm)
Water, Health: $15 \times 4.35 \times 10^5 = 6.5 \times 10^6$ μg/ℓ
Land, Health: $0.2 \times 6.5 \times 10^6 = 1.3 \times 10^6$ μg/g

Air, Ecology:
Water, Ecology: $100 \times 10 = 1{,}000$ μg/l
Land, Ecology: $0.2 \times 1{,}000 = 200$ μg/g

* **ESTIMATED PERMISSIBLE CONCENTRATIONS:**

$EPC_{AH2} = 10^3\ 435/420 = 1{,}040$ μg/m^3
$EPC_{AH3} = 100/420 = 0.24$ ppm
$EPC_{WH1} = 15 \times 1{,}040 = 15{,}600$ μg/ℓ
$EPC_{WH2} = 13.8 \times 435 = 6{,}000$ μg/ℓ
$EPC_{LH} = 0.2 \times 6{,}000 = 1{,}200$ μg/g

$EPC_{WE1} = 50 \times 10 = 500$ μg/l
$EPC_{LH} = 0.2 \times <500 = 100$ μg/g

*Based on TLV for xylenes because of toxicological similarity.

MULTIMEDIA ENVIRONMENTAL GOALS

15B100
DIALKYL BENZENES (MW: 134-191)

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			4.35E5		1,040 (0.24)		
Water, $\mu g/l$ (ppm Wt)			6.5E6	1.0E3	6,000	500	1.0 †
Land, $\mu g/g$ (ppm Wt)			1.3E6	2.0E2	1,200	100	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			1,040 (0.24)		
Water, $\mu g/l$ (ppm Wt)			6,000	500	
Land, $\mu g/g$ (ppm Wt)			1,200	100	

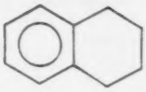
†Highest concentration reported in drinking water.

CATEGORY: 15B

WLN: L66+TJ

TETRAHYDRONAPHTHALENE: $C_{10}H_{12}$ (tetralin, tetraline).
A colorless liquid; menthol odor. 15B120

STRUCTURE:



PROPERTIES:

Molecular Wt.: 132.2; mp: -35.79; bp: 207.57, 79.36^{10}; d: 0.9707_4^{20}; vap. press: 1 mm at 38°; vap. d: 4.55; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Tetrahydronaphthalene is produced by the catalytic hydrogenation of naphthalene (ref. 8). It is used as a solvent and has been used as a larvacide for mosquitoes (ref. 10).

In the presence of selenium or sulfur, the compound may dehydrogenate to give naphthalene and H_2S or H_2Se.

TOXIC PROPERTIES, HEALTH EFFECTS:

Tetrahydronaphthalene is an irritant in low concentrations. Narcotic effects result from exposure to high concentrations (ref. 7). Dermatitis has also resulted from exposure (ref. 10).

LD_{50} (oral, rat): 2,860 mg/kg (ref. 14).

LC_{Lo} (inhalation, guinea pig): 275 ppm for 8 hours for 17 days (ref. 14).

Aquatic toxicity: TLm96: 100-10 ppm (ref. 14).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 2860 = 1.3 \times 10^5$ μg/m³

Water, Health: $15 \times 1.3 \times 10^5 = 2.0 \times 10^6$ μg/ℓ

Land, Health: $0.2 \times 2.0 \times 10^6 = 4.0 \times 10^5$ μg/g

Air, Ecology:

Water, Ecology: $100 \times 10 = 1.0 \times 10^3$ μg/ℓ

Land, Ecology: $0.2 \times 1.0 \times 10^3 = 200$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 2,860 = 306$ μg/m³

$EPC_{AH3} = 0.081 \times 2,860 = 232$ μg/m³

$EPC_{WH1} = 15 \times 232 = 3,480$ μg/ℓ

$EPC_{WH2} = 0.4 \times 2,860 = 1,140$ μg/ℓ

$EPC_{LH} = 0.2 \times 1,140 = 230$ μg/g

$EPC_{WE1} = 50 \times 10 = 500$ μg/ℓ

$EPC_{LE} = 0.2 \times 500 = 100$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

15B120
TETRAHYDRONAPHTHALENE

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)			1.3E5		232		
Water, μg/l (ppm Wt)			2.0E6	1.0E3	1,140	500	
Land, μg/g (ppm Wt)			4.0E5	2.0E2	230	100	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)			232		
Water, μg/l (ppm Wt)			1,140	500	
Land, μg/g (ppm Wt)			230	100	

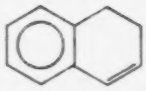
CATEGORY: 15B

WLN: L66BUT&J

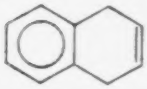
DIHYDRONAPHTHALENES: 15B140

1,2-DIHYDRONAPHTHALENE. $C_{10}H_{10}$. A liquid. 15B141
1,4-DIHYDRONAPHTHALENE. $C_{10}H_{10}$. A solid or liquid. 15B142

STRUCTURE:



1,2-dihydronaphthalene



1,4-dihydronaphthalene

PROPERTIES:

1,2-dihydronaphthalene: mol. wt: 130.19; mp: -8 to -7; bp: 206-7; d: 0.9974_4^{20}; insoluble in water.

1,4-dihydronaphthalene: mol. wt: 130.19; mp: 25; bp: $211\text{-}2^{760}$; d: 0.9928_4^{33}; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

In the presence of sulfur or selenium, the dihyrdonaphthalenes may form naphthalene and H_2S or H_2Sr.

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{50} (oral, rat): 2,830 mg/kg for 1,2-dihydronaphthalene (ref. 14).

Toxic properties are probably similar to those of tetrahydronaphthalenes.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$45 \times 2{,}830 = 1.27 \times 10^5\ \mu g/m^3$	Air, Ecology:
Water, Health:	$15 \times 1.27 \times 10^5 = 1.91 \times 10^6\ \mu g/l$	Water, Ecology:
Land, Health:	$0.2 \times 1.91 \times 10^6 = 3.8 \times 10^5\ \mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 2{,}830 = 302.8\ \mu g/m^3$

$EPC_{AH3} = 0.081 \times 2{,}830 = 229.2\ \mu g/m^3$

$EPC_{WH1} = 15 \times 229.2 = 3{,}438\ \mu g/l$

$EPC_{WH2} = 0.4 \times 2{,}830 = 1{,}132\ \mu g/l$

$EPC_{LH} = 0.2 \times 1{,}132 = 226\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

15B140
DIHYDRONAPHTHALENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.27E5		229		
Water, $\mu g/l$ (ppm Wt)			1.91E6		1,132		
Land, $\mu g/g$ (ppm Wt)			3.8E5		226		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			229		
Water, $\mu g/l$ (ppm Wt)			1,132		
Land, $\mu g/g$ (ppm Wt)			226		

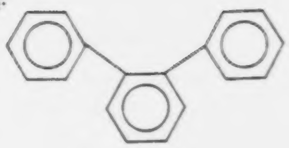
CATEGORY: 15B

TERPHENYLS: $(C_6H_5)_2\ C_6H_4$ 15B160

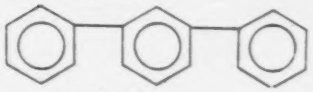
o-TERPHENYL: (1,2-diphenylbenzene). A solid or liquid. 15B161
m-TERPHENYL: (1,3-diphenylbenzene). Colorless needles. 15B162
p-TERPHENYL: (1,4-diphenylbenzene). A solid. 15B163

WLN:

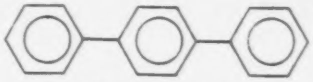
STRUCTURE:



o-terphenyl



m-terphenyl



p-terphenyl

PROPERTIES:

	mol.wt.	mp.	bp.	d.	vap.d.	water solubility
o-terphenyl	230.31	58	332^{760}	1.14	7.95	insoluble
m-terphenyl	230.31	89	365^{760}	1.164	7.95	insoluble
p-terphenyl	230.31	213	405	1.236	7.95	insoluble

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Terphenyls are used as heat-exchange fluids and as atomic reactor moderator coolants (ref. 9). Terphenyls have been reported in samples of finished drinking water (ref. 12). Polychlorinated terphenyls are expected to be found in seawater and in marine organisms: trophic accumulation is also expected (ref. 13).

TOXIC PROPERTIES, HEALTH EFFECTS:

Workers exposed to dust and vapor experienced marked irritation at concentrations in air above 10 mg/m^3 (ref. 9). Terphenyls may produce eye, skin, and respiratory irritation and may cause sensitization, but this has not been demonstrated with humans (ref. 9).

Of the 3 isomers, o-terphenyl has been demonstrated to be the most toxic on ingestion (ref. 9).

In general, the terphenyls do not present industrial hygiene hazards due to their low vapor pressure and low order of toxicity (ref. 10).

LD_{Lo} (oral, rat): 500 mg/kg for p-terphenyl (ref.14).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 9 mg/m^3 (1 ppm)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$10^3 \times 9 = 9{,}000\ \mu g/m^3$ (1 ppm)	Air, Ecology:
Water, Health:	$15 \times 9 \times 10^3 = 1.35 \times 10^5\ \mu g/l$	Water, Ecology:
Land, Health:	$0.2 \times 1.35 \times 10^5 = 2.7 \times 10^4\ \mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 9/420 = 21.4\ \mu g/m^3$

$EPC_{AH1a} = 1/420 = 2.38 \times 10^{-3}$ ppm

$EPC_{WH1} = 15 \times 21.4 = 321\ \mu g/l$

$EPC_{WH2} = 13.8 \times 9 = 124\ \mu g/l$

$EPC_{LH} = 0.2 \times 124 = 25\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

15B160 TERPHENYLS

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			9.0E3 (1)		21 (0.002)		
Water, $\mu g/l$ (ppm Wt)			1.35E5		124		
Land, $\mu g/g$ (ppm Wt)			2.7E4		25		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			21 (0.002)		
Water, $\mu g/l$ (ppm Wt)			124		
Land, $\mu g/g$ (ppm Wt)			25		

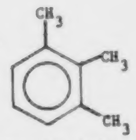
CATEGORY: 15B

TRIMETHYLBENZENES: $(CH_3)_3\ C_6H_3$. 15B180
1,2,3-TRIMETHYLBENZENE: (hemimellitene). 15B181
1,2,4-TRIMETHYLBENZENE: (pseudocumene). 15B182
1,3,5-TRIMETHYLBENZENE: (mesitylene). 15B183
All are colorless liquids.

WLN:

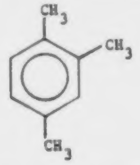
STRUCTURE:

IR BCC/



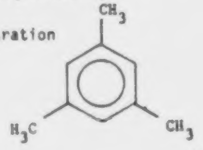
(1,2,3-trimethylbenzene)

IR B D/



(1,2,4-trimethylbenzene)

IR C E/



(1,3,5-trimethylbenzene)

PROPERTIES:

	mol.wt.	mp.	bp.	d.	water solubility
1,2,3-Trimethylbenzene	120.20	-25.4	176.1	0.8944	insoluble
1,2,4-Trimethylbenzene	120.20	-43.8	169.4	0.8758	insoluble
1,3,5-Trimethylbenzene	120.20	-44.7	164.7	0.8652	insoluble

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Rural background concentrations of trimethylbenzenes are reported as follows (ref. 5).

Chemical	Rural Concentration
1,2,4-trimethylbenzene	2.7 - 97 ppbc (1.47 - 52.9 μg/m³)
1,3,5-trimethylbenzene	0.01 - 21 ppbc (0.005 - 11.4 μg/m³)

Trimethylbenzenes have also been found in drinking water, with the highest reported concentration at 6.1 μg/l (ref. 6).

Trimethybenzenes occur in coal tar and in petroleum crudes (ref. 8).

TOXIC PROPERTIES, HEALTH EFFECTS:

Trimethylbenzenes may act as a CNS depressant and a respiratory irritant (ref. 8). Workers exposed to 1,2,4- and 1,3,5-trimethylbenzene at 10-60 ppm for several years exhibited nervousness, tension and asthmatic bronchitis (ref. 15).

Chemical	LD_{Lo} (oral, rat) (mg/kg)	LC_{Lo} (inhalation, rat)
1,2,3-Trimethylbenzene	5,000	
1,2,4-Trimethylbenzene	5,000	
1,3,5-Trimethylbenzene		2,400 ppm for 24 hrs.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 120 mg/m³ (25 ppm) established for trimethylbenzene mixture or individual isomers.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $10^3 \times 120 = 1.2 \times 10^5$ μg/m³ (25 ppm)
Water, Health: $15 \times 1.2 \times 10^5 = 1.8 \times 10^6$ μg/l
Land, Health: $0.2 \times 1.8 \times 10^6 = 3.6 \times 10^5$ μg/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 120/420 = 285.7$ μg/m³

$EPC_{AH1a} = 25/420 = 0.06$ ppm

$EPC_{WH1} = 15 \times 285.7 = 4{,}286$ μg/l

$EPC_{WH2} = 13.8 \times 120 = 1{,}656$ μg/l

$EPC_{LH} = 0.2 \times 1{,}656 = 331$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

15B180
TRIMETHYLBENZENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.2E5 (25)		286 (0.06)		0.005 - 53
Water, $\mu g/l$ (ppm Wt)			1.8E6		1,656		6.1†
Land, $\mu g/g$ (ppm Wt)			3.6E5		331		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			286 (0.06)		
Water, $\mu g/l$ (ppm Wt)			1,656		
Land, $\mu g/g$ (ppm Wt)			331		

†Highest concentration reported in drinking water.

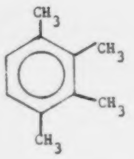
CATEGORY: 15B

TETRAMETHYLBENZENES: $(CH_3)_4\ C_6H_2$ 15B200

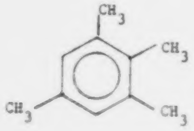
1,2,3,4-TETRAMETHYLBENZENE. (prehnitene). A liquid. 15B201
1,2,3,5-TETRAMETHYLBENZENE. (isodurene). A liquid. 15B202
1,2,4,5-TETRAMETHYLBENZENE. (durene). A solid. 15B203

WLN:

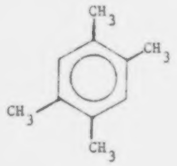
STRUCTURE:



(1,2,3,4-tetramethylbenzene)



(1,2,3,5-tetramethylbenzene)



(1,2,4,5-tetramethylbenzene)

PROPERTIES:

	mol.wt.	mp.	bp.	d.	water solubility
1,2,3,4-Tetramethylbenzene	134.22	-6.25	205	0.9052	insoluble
1,2,3,5-Tetramethylbenzene	134.22	-23.68	198	0.8903	insoluble
1,2,4,5-Tetramethylbenzene	134.22	79.24	196.8	0.8875	insoluble

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Tetramethylbenzene isomers have been reported in samples taken from finished drinking water (ref. 12). The highest concentration reported has been less than 1.0 μg/l (ref. 6).

Tetramethylbenzene isomers are found in coal tars (ref. 8).

TOXIC PROPERTIES, HEALTH EFFECTS:

The toxicity of the tetramethylbenzenes is probably similar to that of the trimethyl benzenes.

Aquatic toxicity: TLm 96: 1,000 = 100 ppm for a mixture of isomers (ref. 14).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV for trimethylbenzenes: 120 mg/m^3 (25 ppm).

*MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $10^3 \times 120 = 1.2 \times 10^5$ μg/m^3 (25 ppm)	Air, Ecology:
Water, Health: $15 \times 1.2 \times 10^5 = 1.8 \times 10^6$ μg/l	Water, Ecology: $100 \times 100 = 1.0 \times 10^4$ μg/l
Land, Health $0.2 \times 1.8 \times 10^6 = 3.6 \times 10^5$ μg/g	Land, Ecology: $0.2 \times 1.0 \times 10^4 = 2.0 \times 10^3$ μg/g

*ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 120/420 = 285.7$ μg/m^3

$EPC_{AH1a} = 25/420 = 0.06$ ppm

$EPC_{WH1} = 15 \times 285.7 = 4,286$ μg/l

$EPC_{WH2} = 13.8 \times 120 = 1,656$ μg/l

$EPC_{LH} = 0.2 \times 1,656 = 331$ μg/g

$EPC_{WE1} = 50 \times 100 = 5,000$ μg/l

$EPC_{LE} = 0.2 \times 5,000 = 1,000$ μg/g

*Health based values derived from TLV for trimethylbenzenes.

15B200
TETRAMETHYLBENZENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			1.2E5		286 (0.06)		
Water, μg/l (ppm Wt)			1.8E6	1.0E4	1,656	5,000	< 1.0†
Land, μg/g (ppm Wt)			3.6E5	2.6E3	331	1,000	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			286 (0.06)		
Water, μg/l (ppm Wt)			1,656	5,000	
Land, μg/g (ppm Wt)			331	1,000	

†Highest concentration reported in finished drinking water.

REFERENCES: CATEGORY 15B

Benzene, Substituted Benzene Hydrocarbons - Disubstituted and Polysubstituted Benzene Hydrocarbons

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14. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

15. National Academy of Sciences, National Research Council. Vapor-Phase Organic Pollutants: Medical and Biological Effects of Environmental Pollutants. National Academy of Science, Washington, DC (1976).

16. Mattson, V. R., J. W. Arthur, and C. G. Walbridge. Acute Toxicity of Selected Compounds to Fathead Minnows. U.S. Environmental Protection Agency, Office of Research and Development, Duluth, MN. EPA-600/3-76-097 (1976).

CATEGORY 16

HALOGENATED AROMATIC COMPOUNDS

SUBCATEGORY: 16A - Ring Substituted Aromatics

Summary of Subcategory

Total number of compounds in subcategory	17
number of parent compounds with subspecies	4
number of subspecies	10
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	2

Consent Decree compounds included in subcategory: 9

16A020	Chlorobenzene
16A100	1,2-Dichlorobenzene
16A120	1,3-Dichlorobenzene
16A140	1,4-Dichlorobenzene
16A161	1,2,4-Trichlorobenzene
16A162	Hexachlorobenzene
16A201	1-Chloronaphthalene
16A202	2-Chloronaphthalene
16A220	Polychlorinated biphenyls

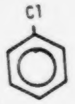
CATEGORY: 16A

CHLOROBENZENE: C_6H_5Cl (phenyl chloride). 16A020

A colorless liquid, faint, not unpleasant odor.

WLN: GR

STRUCTURE:



PROPERTIES:

Molecular wt: 112.56; mp: -45.6; bp: 131-132;
d: 1.1058; vap. d: 3.88; vap. press: 10 mm at 22°; solubility in water: 49 mg/100 ml at 20°C.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Odor threshold level for chlorobenzene is reported as 0.21 ppm (ref. 1). Chlorobenzene has been found in samples of U.S. drinking water supplies at levels of less than 5 μg/ℓ (ref. 2).

TOXIC PROPERTIES, HEALTH EFFECTS:

Chlorobenzene is a central nervous system depressant and may affect the liver and kidneys (ref. 3). It has only slight irritant qualities (ref. 4).

A narcotic effect was observed when animals were exposed to concentrations of chlorobenzene above 1,200 ppm (ref. 5). Little information is available on human effects from repeated exposure to subnarcotic concentrations (ref. 4).

LD_{50} (oral, rat): 2,910 mg/kg.
Aquatic toxicity: TLm96: 100-1 ppm (ref. 6).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 350 mg/m^3 (75 ppm).
Chlorobenzene is on EPA Consent Decree Priority 2 List.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 3.50×10^5 μg/m^3 (75 ppm)
Water, Health: $15 \times 3.5 \times 10^5 = 5.25 \times 10^6$ μg/ℓ
Land, Health: $0.2 \times 5.25 \times 10^6 = 1.05 \times 10^6$ μg/g

Air, Ecology:
Water, Ecology: $100 \times 1 = 100$ μg/ℓ
Land, Ecology: $0.2 \times 100 = 20$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 350/420 = 830$ μg/m^3
$EPC_{AH1a} = 75/420 = 0.18$ ppm
$EPC_{WH1} = 15 \times 830 = 12{,}500$ μg/ℓ
$EPC_{WH2} = 13.8 \times 350 = 4{,}830$ μg/ℓ
$EPC_{LH} = 0.2 \times 4{,}830 = 9.66 \times 10^2$ μg/g

$EPC_{WE1} = 50 \times 1 = 50$ μg/ℓ
$EPC_{LE} = 0.2 \times 50 = 10$ μg/g

16A020
CHLOROBENZENE

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			3.50E5 (75)		830 (0.18)		
Water, μg/l (ppm Wt)			5.25E6	1.0E2	4,830	50	<5[+]
Land, μg/g (ppm Wt)			1.05E6	2.0E1	966	10	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			830 (0.18)		
Water, μg/l (ppm Wt)			4,830	50	
Land, μg/g (ppm Wt)			966	10	

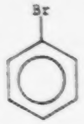
[+] Drinking water supplies.

CATEGORY: 16A

BROMOBENZENE: C_6H_5Br (phenyl bromide).
A colorless liquid with an aromatic odor. 16A040

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 157.02; mp: -30.82; bp: 156; d: 1.4950;
vap.d: 5.41; vap.press: 10 mm at 40°; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Bromobenzene has been reported in samples taken from finished drinking water and from river water in the U.S. (ref. 7).

Bromobenzene is used as a solvent on a large scale and where a heavy liquid is desirable. It is also used as a motor oil additive, and in the manufacture of phenyl magnesium bromide (ref. 8).

TOXIC PROPERTIES, HEALTH EFFECTS:

Bromobenzene is reported as being irritating to the skin (ref. 8). When heated to decomposition, bromobenzenes may produce toxic fumes of bromides (ref. 4). Toxicological data for bromobenzene are not available. However, toxicological characteristics of bromobenzene are likely to be similar to those of chlorobenzene. Data for chlorobenzene from ref. 6 are shown below.

Chemical	TLV (mg/m^3)	TLV (ppm)	LD^{50} (oral, rat) (mg/kg)	Aquatic toxicity (ppm)
monochlorobenzene	350	75	2,910	100-1

Data from aliphatic compounds indicate that chlorine substitution increases toxicity more than bromine substitution.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 350 mg/m^3 (75 ppm) for monochlorobenzene.

*MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $4.88 \times 10^5\ \mu g/m^3$ (75 ppm)

Water, Health: $15 \times 4.88 \times 10^5 = 7.32 \times 10^6\ \mu g/l$

Land, Health: $0.2 \times 7.32 \times 10^6 = 1.46 \times 10^6\ \mu g/g$

Air, Ecology:

Water, Ecology: $100 \times 1 = 100\ \mu g/l$

Land, Ecology: $0.2 \times 100 = 20\ \mu g/g$

*ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 488/420 = 1{,}161\ \mu g/m^3$

$EPC_{AH1a} = 75/420 = 0.18$ ppm

$EPC_{WH1} = 15 \times 1{,}161 = 1.74 \times 10^4\ \mu g/l$

$EPC_{WH2} = 13.8 \times 488 = 6{,}734\ \mu g/l$

$EPC_{LH} = 0.2 \times 6{,}734 = 1.346 \times 10^3\ \mu g/g$

$EPC_{WE1} = 50 \times 1 = 50\ \mu g/l$

$EPC_{LE} = 0.2 \times 50 = 10\ \mu g/g$

*Based on TLV for monochlorobenzene; molecular wt. ratio = $\frac{157.02\ \text{(bromobenzene)}}{112.56\ \text{(monochlorobenzene)}} = 1.395$

MULTIMEDIA ENVIRONMENTAL GOALS

16A040
BROMOBENZENE

EMISSION LEVEL GOALS †

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			4.88E5 (75)		1,161 (0.18)		
Water, μg/l (ppm Wt)			7.32E6	1.0E2	6,734	50	
Land, μg/g (ppm Wt)			1.46E6	2.0E1	1,346	10	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS†

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			1,161 (0.18)		
Water, μg/l (ppm Wt)			6,734	50	
Land, μg/g (ppm Wt)			1,346	10	

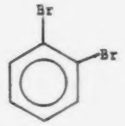
†Based on data for chlorobenzene.

CATEGORY: 16A

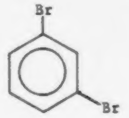
WLN:

DIBROMOBENZENES: 16A060
1,2-DIBROMOBENZENE: $C_6H_4Br_2$. A colorless liquid. 16A061
1,3-DIBROMOBENZENE: $C_6H_4Br_2$. A colorless liquid. 16A062
1,4-DIBROMOBENZENE: $C_6H_4Br_2$. A colorless liquid with the odor of xylene. 16A063

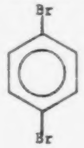
STRUCTURE:



(1,2-dibromobenzene)



(1,3-dibromobenzene)



(1,4-dibromobenzene)

PROPERTIES:

	mol.wt.	mp	bp	d	vap.d.	vap.press.	water solubility
1,2-dibromobenzene	235.92	7.1	225	1.9843			insoluble
1,3-dibromobenzene	235.92	-7	218	1.9523			insoluble
1,4-dibromobenzene	235.92	87.33	218-9	1.8322_4^{100}	8.1	1 mm at 61°	insoluble

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Dibromobenzene isomers have been reported in samples taken from finished drinking water and from river water in the U.S. (ref. 7).

TOXIC PROPERTIES, HEALTH EFFECTS:

Bromobenzenes are reported to be irritating to the skin (ref. 8). When heated to decomposition, bromobenzenes may produce toxic fumes of bromides (ref. 4). Toxicological data for dibromobenzenes are not available. However, toxicological characteristics of dibromobenzenes are likely to be similar to those of dichlorobenzenes. Data for dichlorobenzenes from ref. 6 are shown below.

Chemical	TLV		LD_{50} (oral, rat)	Aquatic toxicity
	(mg/m³)	(ppm)	(mg/kg)	(ppm)
1,2-dichlorobenzene	300	50	--	10 to <1 (for mixed isomers)
1,3-dichlorobenzene	--	--	--	
1,4-dichlorobenzene	450	75	500	

Data from aliphatic compounds indicate that chlorine substitution increases toxicity more than bromine substitution.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 300 mg/m³ (50 ppm) for 1,2-dichlorobenzene.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 4.81×10^5 μg/m³ (50 ppm)
Water, Health: $15 \times 4.81 \times 10^5 = 7.22 \times 10^6$ μg/l
Land, Health: $0.2 \times 7.22 \times 10^6 = 1.44 \times 10^6$ μg/g

Air, Ecology:
Water, Ecology: $100 \times 1 = 100$ μg/l
Land, Ecology: $0.2 \times 100 = 20.0$ μg/g

***ESTIMATED PERMISSIBLE CONCENTRATIONS:**

$EPC_{AH1} = 10^3 \times 481/420 = 1{,}145$ μg/m³
$EPC_{AH1a} = 50/420 = 0.12$ ppm
$EPC_{WH1} = 15 \times 1{,}145 = 1.72 \times 10^4$ μg/l
$EPC_{WH2} = 13.8 \times 481 = 6{,}638$ μg/l
$EPC_{LH} = 0.2 \times 6{,}638 = 1.328 \times 10^3$ μg/g

$EPC_{WE1} = 50 \times 1 = 50$ μg/l
$EPC_{LE} = 0.2 \times 50 = 10$ μg/g

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*Based on TLV for 1,2-dichlorobenzene; molecular weight ratio = $\frac{235.92 \text{ (dibromobenzene)}}{147.01 \text{ (dichlorobenzene)}} = 1.605$

MULTIMEDIA ENVIRONMENTAL GOALS

16A060 DIBROMOBENZENES

EMISSION LEVEL GOALS†

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			4.81E5		1,145 (0.12)		
Water, μg/l (ppm Wt)			7.22E6	1.0E2	6,638	50	
Land, μg/g (ppm Wt)			1.44E6	2.0E1	1,328	10	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS †

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			1,145 (0.12)		
Water, μg/l (ppm Wt)			6,638	50	
Land, μg/g (ppm Wt)			1,328	10	

†Based on data for dichlorobenzenes.

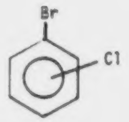
CATEGORY: 16A

BROMOCHLOROBENZENES: C_6H_4BrCl. 16A080

1-BROMO-2-CHLOROBENZENE: A liquid. 16A081
1-BROMO-3-CHLOROBENZENE: A liquid. 16A082
1-BROMO-4-CHLOROBENZENE: A solid. 16A083

WLN:

STRUCTURE:



PROPERTIES:

	mol.wt.	mp.	bp.	d.	water solubility
1-bromo-2-chlorobenzene	191.46	-12.3	204	1.6382	insoluble
1-bromo-3-chlorobenzene	191.46	-21.5	196	1.6302	insoluble
1-bromo-4-chlorobenzene	191.46	68	196	1.576	insoluble

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Bromochlorobenzene isomers have been reported in samples taken from finished drinking water in the U.S. (ref. 7).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for bromobenzenes are not available at this time. However, toxicological characteristics of bromochlorobenzenes are likely to be similar to those of dichlorobenzenes. Data for dichlorobenzenes from ref. 6 are shown below.

Chemical	TLV		LD_{50} (oral, rat)	Aquatic toxicity
	(mg/m^3)	(ppm)	(mg/kg)	(ppm)
monochlorobenzene	350	75	2,910	100-1
1,2-dichlorobenzene	300	50	--	
1,3-dichlorobenzene	--	--	--	10 to <1 (for mixed isomers)
1,4-dichlorobenzene	450	75	500	

Data from aliphatic compounds indicates that chlorine substitution increases toxicity more than bromine substitution.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 300 mg/m^3 (50 ppm) for 1,2-dichlorobenzene.

*** MINIMUM ACUTE TOXICITY CONCENTRATIONS:**

Air, Health: 3.91×10^5 µg/m^3 (50 ppm)
Water, Health: $15 \times 3.91 \times 10^5 = 5.87 \times 10^6$ µg/l
Land, Health: $0.2 \times 5.87 \times 10^6 = 1.17 \times 10^6$ µg/g

Air, Ecology:
Water, Ecology: $100 \times 1 = 100$ µg/l
Land, Ecology: $0.2 \times 100 = 20$ µg/g

***ESTIMATED PERMISSIBLE CONCENTRATIONS:**

$EPC_{AH1} = 10^3 \times 391/420 = 931$ µg/m^3
$EPC_{AH1a} = 50/420 = 0.12$ ppm
$EPC_{WH1} = 15 \times 931 = 1.40 \times 10^4$ µg/l
$EPC_{WH2} = 13.8 \times 391 = 5.40 \times 10^3$ µg/l
$EPC_{LH} = 0.2 \times 5.40 \times 10^3 = 1.08 \times 10^3$ µg/g

$EPC_{WE1} = 50 \times 1 = 50$ µg/l
$EPC_{LE} = 0.2 \times 50 = 10$ µg/g

*Based on TLV for 1,2-dichlorobenzene; molecular wt ratio = $\frac{191.46 \text{ (bromochlorobenzene)}}{147.01 \text{ (dichlorobenzene)}} = 1.302$

MULTIMEDIA ENVIRONMENTAL GOALS

16A080
BROMOCHLOROBENZENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			3.91E5 (50)		931 (0.12)		
Water, $\mu g/l$ (ppm Wt)			5.87E6	1.0E2	5,400	50	
Land, $\mu g/g$ (ppm Wt)			1.17E6	2.0E1	1,080	10	

*To be multiplied by dilution factor

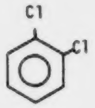
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			931 (0.12)		
Water, $\mu g/l$ (ppm Wt)			5,400	50	
Land, $\mu g/g$ (ppm Wt)			1,080	10	

CATEGORY: 16A

WLN: GR BG

1,2-DICHLOROBENZENE: $C_6H_4Cl_2$, (o-dichlorobenzene). 16A100
A colorless liquid.

STRUCTURE:



PROPERTIES:

Molecular wt: 147.01; mp: -17; bp: 180; d: 1.3048; Vap. d: 5.07; vap. press: 1.56 mm at 25°; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

The odor of o-dichlorobenzene may be detected at 50 ppm (300 mg/m^3) (ref. 3).

o-Dichlorobenzene has been found in samples of U.S. drinking water supplies in a concentration of 1 μg/ℓ (ref. 2).

The compound is not known to occur in nature. It is produced commercially and used as a solvent and as a chemical intermediate (ref. 12).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicity of 1,2-Dichlorobenzene is similar to that of other aromatic chloro compounds; however, the o-isomer of dichlorobenzene is somewhat more toxic than the m- or p-forms. It causes central nervous system depression, can injure the liver and kidneys, and is irritating to skin and mucous membranes (ref. 4). Exposure to concentrations above 90 ppm affected test animals (ref. 5).

LC_{Lo} (inhalation, rat): 707 ppm for 7 hours.

LD_{Lo} (oral, guinea pig): 2,000 mg/kg.

Aquatic toxicity: 96-hr TLm (for mixed dichlorobenzene isomers): 10 to < 1 ppm (ref. 6).

A concentration of 0.25 mg/ℓ of 1,2-Dichlorobenzene is reported to cause tainting of fish flesh (ref. 9).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 300 mg/m^3 (50 ppm).

On EPA Consent Decree Priority I List.

1,2-Dichlorobenzene has been reviewed by the International Agency for Research on Cancer. They concluded that there is insufficient evidence to indicate carcinogenic risk from the compound (ref. 12).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 3.0×10^5 μg/m^3 (50 ppm)
Water, Health: $15 \times 3 \times 10^5 = 4.5 \times 10^6$ μg/ℓ
Land, Health: $0.2 \times 4.5 \times 10^6 = 9.0 \times 10^5$ μg/g

Air, Ecology:
Water, Ecology: $100 \times 1 = 100$ μg/ℓ
Land, Ecology: $0.2 \times 100 = 20$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 300/420 = 714$ μg/m^3
$EPC_{AH1a} = 50/420 = 0.12$ ppm
$EPC_{WH1} = 15 \times 714 = 10{,}700$ μg/ℓ
$EPC_{WH2} = 13.8 \times 300 = 4{,}140$ μg/ℓ
$EPC_{LH} = 0.2 \times 4{,}140 = 828$ μg/g

$EPC_{WE1} = 50 \times 1 = 50$ μg/ℓ
$EPC_{WE2} = 250$ μg/ℓ
$EPC_{LE} = 0.2 \times 50 = 10$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

16A100
1,2-DICHLOROBENZENE

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			3.0E5 (50)		714 (0.12)		
Water, $\mu g/l$ (ppm Wt)			4.5E6	1.0E2	4,140	50	1†
Land, $\mu g/g$ (ppm Wt)			9.0E5	2.0E1	828	10	

*To be multiplied by dilution factor

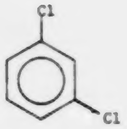
	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			714 (0.12)		
Water, $\mu g/l$ (ppm Wt)			4,140	50	
Land, $\mu g/g$ (ppm Wt)			828	10	

†Drinking water supplies.

CATEGORY: 16A
1,3-DICHLOROBENZENE: $C_6H_4Cl_2$ (m-dichlorobenzene).
A colorless liquid. 16A120

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 147.01; mp: -24.7; bp: 173; d: 1.2884;
vap. d: 5.08; vap. press: 1mm at 12.1°; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

1,3-Dichlorobenzene has been reported in samples taken from river water, well water, raw public water supplies, and finished drinking water in the U.S. (ref. 7). The highest reported concentration in drinking water is reported as less than 3.0 μg/l (ref. 2).

1,3-Dichlorobenzene is used as an insecticide and fumigant (ref. 4).

TOXIC PROPERTIES, HEALTH EFFECTS:

1,3-Dichlorobenzene is believed to be less toxic than the ortho-isomer (ref. 4).
LC_{Lo} (rat): 707 ppm for 7 hours for 1,2-Dichlorobenzene (ref. 6).
LD_{Lo} (oral, guinea pig): 2,000 mg/kg for 1,2-Dichlorobenzene (ref. 6).
Aquatic toxicity: TLm 96: 10- under 1 ppm for mixed isomers (ref. 6).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

1,3-Dichlorobenzene is on the EPA Consent Decree List, Priority 1.
TLV = 300 mg/m³ (50 ppm) for 1,2-Dichlorobenzene.

* **MINIMUM ACUTE TOXICITY CONCENTRATIONS**:

Air, Health: 3.0×10^5 μg/m³ (50 ppm)
Water, Health: $15 \times 3.0 \times 10^5 = 4.5 \times 10^6$ μg/l
Land, Health: $0.2 \times 4.5 \times 10^6 = 9.0 \times 10^5$ μg/g

Air, Ecology:
Water, Ecology: $100 \times <1 = <100$ μg/l
Land, Ecology: $0.2 \times <100 = <20$ μg/g

* **ESTIMATED PERMISSIBLE CONCENTRATIONS**:

$EPC_{AH1} = 10^3 \times 300/420 = 714$ μg/m³
$EPC_{AH1a} = 50/420 = 0.12$ ppm
$EPC_{WH1} = 15 \times 714 = 10,700$ μg/l
$EPC_{WH2} = 13.8 \times 300 = 4,140$ μg/l
$EPC_{LH} = 0.2 \times 4,140 = 8.28 \times 10^2$ μg/g

$EPC_{WE1} = 50 \times < 1 = < 50$ μg/l
$EPC_{LE} = 0.2 \times < 50 = <10$ μg/g

* Health values based on TLV for 1,2-Dichlorobenzene

MULTIMEDIA ENVIRONMENTAL GOALS

16A120
1,3-DICHLOROBENZENE

EMISSION LEVEL GOALS†

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)			3.0E5		714 (0.12)		
Water, μg/l (ppm Wt)			4.5E6	1.0E2	4,140	50	<3.0‡
Land, μg/g (ppm Wt)			9.0E5	2.0E1	828	<10	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS†

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)			714 (0.12)		
Water, μg/l (ppm Wt)			4,140	50	
Land, μg/g (ppm Wt)			828	10	

†Based on data for 1,2-Dichlorobenzene.

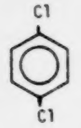
‡Highest concentration reported in drinking water.

CATEGORY: 16A

WLN: GR DG

1,4-DICHLOROBENZENE: $C_6H_4Cl_2$ (p-Dichlorobenzene). 16A140
Volatile crystals with characteristic, penetrating odor.

STRUCTURE:



PROPERTIES:

Molecular wt: 147.01; mp: 53; bp: 174; d: 1.2884; vap. d: 5.07; vap. press: 10 mm at 55°; insoluble in water; sublimes at ordinary temperatures.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

The odor threshold level is 15-30 ppm (90-180 mg/m^3) in air (ref. 3). 1,4-Dichlorobenzene has been found in a concentration of 1 μg/ℓ in samples of U.S. drinking water supplies (ref. 2). The compound is not known to occur in nature (ref. 12). It is manufactured and used widely as an insecticide, disinfectant, and chemical intermediate (ref. 3).

TOXIC PROPERTIES, HEALTH EFFECTS:

Vapors of 1,4-dichlorobenzene can cause irritation to skin, throat, and eyes; repeated exposure to high concentrations may cause liver injury and central nervous system depression (refs. 8,3). Ingestion of 300 mg/kg by a human has resulted in unspecified toxic effects (ref. 6). The compound is indicated to be less toxic than 1,2-dichlorobenzene (ref. 5).

LD_{50} (oral, rat): 500 mg/kg.
Aquatic toxicity: 96-hr. TLm for mixed dichlorobenzene isomers: 10 to <1 ppm (ref. 6)

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 450 mg/m^3 (75 ppm).
On EPA Consent Decree Priority I List.
1,4-Dichlorobenzene has been reviewed by the International Agency for Research on Cancer. They concluded that there is insufficient evidence to indicate carcinogenic risk from this compound (ref. 12).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 4.5×10^5 μg/m^3 (75 ppm)
Water, Health: $15 \times 4.5 \times 10^5 = 6.75 \times 10^6$ μg/ℓ
Land, Health: $0.2 \times 6.75 \times 10^6 = 1.35 \times 10^6$ μg/g

Air, Ecology:
Water, Ecology: $100 \times 1 = 100$ μg/ℓ
Land, Ecology: $0.2 \times 100 = 20$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 450/420 = 1{,}070$ μg/m^3
$EPC_{AH1a} = 75/420 = 0.18$ ppm
$EPC_{WH1} = 15 \times 1{,}070 = 16{,}100$ μg/ℓ
$EPC_{WH2} = 13.8 \times 450 = 6{,}210$ μg/ℓ
$EPC_{LH} = 0.2 \times 6{,}210 = 1.24 \times 10^3$ μg/g

$EPC_{WE1} = 50 \times 1 = 50$ μg/ℓ
$EPC_{LE} = 0.2 \times 50 = 10$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

16A140
1,4-DICHLOROBENZENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			4.5E5 (75)		1,070 (0.18)		
Water, $\mu g/l$ (ppm Wt)			6.75E6	1.0E2	6,210	50	1†
Land, $\mu g/g$ (ppm Wt)			1.35E6	2.0E1	1,240	10	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			1,070 (0.18)		
Water, $\mu g/l$ (ppm Wt)			6,210	50	
Land, $\mu g/g$ (ppm Wt)			1,240	10	

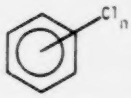
†Drinking water supplies.

CATEGORY: 16A

POLYCHLORINATED BENZENES: 16A160
1,2,4-TRICHLOROBENZENE: $C_6H_3Cl_3$ (unsym-trichlorobenzene).
A colorless liquid; volatile with steam. 16A161
HEXACHLOROBENZENE: C_6Cl_6 (perchlorobenzene). 16A162
A solid.

WLN:

STRUCTURE:



PROPERTIES:
1,2,4-Trichlorobenzene: mol. wt: 181.45; mp. 16.95; bp: 213.5; d: 1.4634; vap. d: 6.26; vap. press: 1 mm at 38.4°; insoluble in water.
Hexachlorobenzene: mol. wt: 284.79; mp. 230; bp: 322 (sublimates); d: 1.5691; vap. d: 9.8; vap. press: 1 mm at 114.4°; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

1,2,4-Trichlorobenzene has been reported in samples taken from raw drinking water in the U.S. (ref. 7). Odor threshold for trichlorobenzene is reported as 3 ppm (ref. 5).

The highest concentration of trichlorobenzene in drinking water reported is 1.0 μg/l (ref. 2). Hexachlorobenzene has also been reported in samples taken from river water and from finished drinking water (ref. 7). Hexachlorobenzene has been detected in birds and is expected to be present in marine organisms (ref. 9).

Hexachlorobenzene is used as a fungicide and in organic syntheses (ref. 8).

TOXIC PROPERTIES, HEALTH EFFECTS:

Studies with rats indicate that trichlorobenzenes are less toxic than the mono- and di-chlorobenzenes. Target organs include the liver, kidney, ganglion cells and mucous membranes (ref. 5).

Chemical	LD_{50} (oral, rat)	Aquatic toxicity TLm 96:
1,2,4-trichlorobenzene	756 mg/kg	10-1 ppm (ref. 6)
hexachlorobenzene	3,500 mg/kg	

Hexachlorobenzene has been shown to produce teratogenic effects in animals (ref. 6). The EPA/NIOSH ordering number based on teratogenicity is 3,111. The lowest dosage reported to produce a teratogenic response is 500 mg/kg. The adjusted ordering number is 6.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 40 mg/m³ (5 ppm) for 1,2,4-Trichlorobenzene.
1,2,4-Trichlorobenzene and hexachlorobenzene are on the EPA Consent Decree List, Priority 2.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/6 = 1.17 \times 10^4$ μg/m³
Water, Health: $15 \times 1.17 \times 10^4 = 1.76 \times 10^5$ μg/l
Land, Health: $0.2 \times 1.76 \times 10^5 = 3.52 \times 10^4$ μg/g

Air, Ecology:
Water, Ecology: $100 \times 1 = 100$ μg/l
Land, Ecology: $0.2 \times 100 = 20$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 40/420 = 95.24$ μg/m³
$EPC_{AH1a} = 5/420 = 0.01$ ppm
$EPC_{WH1} = 15 \times 95.24 = 1{,}429$ μg/l
$EPC_{WH2} = 13.8 \times 40 = 552$ μg/l
$EPC_{LH} = 0.2 \times 552 = 110$ μg/g

$EPC_{WE1} = 50 \times 1 = 50$ μg/l
$EPC_{LE} = 0.2 \times 50 = 10$ μg/g
$EPC_{AT} = 10^3/(6 \times 6) = 27.8$ μg/m³
$EPC_{WT} = 15 \times 27.8 = 417$ μg/ℓ
$EPC_{LT} = 0.2 \times 417 = 83.4$ μg/g

16A160
POLYCHLORINATED BENZENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.17E4		27.8		
Water, $\mu g/l$ (ppm Wt)			1.76E5	1.0E2	417	50	1.0 †
Land, $\mu g/g$ (ppm Wt)			3.52E4	2.0E1	83.4	10	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects ‡
Air, $\mu g/m^3$ (ppm Vol)			95 (0.01)		27.8
Water, $\mu g/l$ (ppm Wt)			552	50	417
Land, $\mu g/g$ (ppm Wt)			110	10	83.4

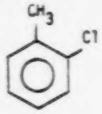
†Highest concentration reported in drinking water.

‡Based on evidence of teratogenicity for hexachlorobenzene.

CATEGORY: 16A

WLN:

STRUCTURE:



2-CHLOROTOLUENE: C_7H_7Cl (o-chlorotoluene, 1-methyl-2-chlorobenzene, o-tolyl chloride). 16A180
A colorless liquid.

PROPERTIES:

Molecular wt: 126.59; mp: -35.1; bp: 159.15; d: 1.0825; vap. press: 10 mm at 46.2°; slightly soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

2-Chlorotoluene is used as a dyestuff intermediate and in organic syntheses (ref. 8).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicity of 2-chlorotoluene is similar to that of other aromatic chloro compounds. Animal exposure to concentrations above 1,000 ppm has resulted in narcotic effects (see ref. 5).

LD_{50} (oral, rat): > 1,600 mg/kg (ref. 5).

Aquatic toxicity: 10 - 1 ppm for p-chlorotoluene (ref. 6).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 250 mg/m^3 (50 ppm) based on analogy with other chlorinated benzenes.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 2.5×10^5 µg/m^3 (50 ppm)	Air, Ecology:
Water, Health: $15 \times 2.5 \times 10^5 = 3.75 \times 10^6$ µg/ℓ	Water, Ecology:
Land, Health: $0.2 \times 3.75 \times 10^6 = 7.5 \times 10^5$ µg/g	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 250/420 = 600$ µg/m^3
$EPC_{AH1a} = 50/420 = 0.12$ ppm
$EPC_{WH1} = 15 \times 600 = 9{,}000$ µg/ℓ
$EPC_{WH2} = 13.8 \times 250 = 3{,}450$ µg/ℓ
$EPC_{LH} = 0.2 \times 3{,}450 = 690$ µg/g

MULTIMEDIA ENVIRONMENTAL GOALS

16A180
2-CHLOROTOLUENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			2.5E5 (50)		600 (0.12)		
Water, μg/l (ppm Wt)			3.75E6		3,450		
Land, μg/g (ppm Wt)			7.5E5		690		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			600 (0.12)		
Water, μg/l (ppm Wt)			3,450		
Land, μg/g (ppm Wt)			690		

CATEGORY: 16A

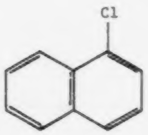
CHLORONAPHTHALENES: $C_{10}H_7Cl$ 16A200

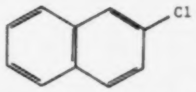
1-CHLORONAPHTHALENE: (α-chloronaphthalene). Oily liquid. 16A201

2-CHLORONAPHTHALENE: (β-chloronaphthalene). A solid. 16A202

WLN:

STRUCTURE:





PROPERTIES:

1-Chloronaphthalene: mol. wt: 162.62; mp: -2.3; bp: 258.8^{753}
d: 1.1938^{20}_{4}; insoluble in water.
2-Chloronaphthalene: mol. wt: 162.62; mp: 61; bp: 256;
d: 1.1377^{71}_{4}; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

1-Chloronaphthalene is used as an immersion liquid in the (microscopic) determination of the refractive index of crystals, and as a solvent for oils, fats, and DDT (ref. 8).

1-Chloronaphthalene can be formed by the reaction between chlorine and boiling naphthalene (ref. 8).

TOXIC PROPERTIES, HEALTH EFFECTS:

Chemical	LD_{50} (oral, rat) (mg/kg)
1-Chloronaphthalene	1,540
2-Chloronaphthalene	2,078

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Chlorinated naphthalene is on the EPA Consent Decree List, Priority 3.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 1{,}540 = 6.93 \times 10^4$ μg/m^3

Water, Health: $15 \times 6.93 \times 10^4 = 1.04 \times 10^6$ μg/l

Land, Health: $0.20 \times 1.04 \times 10^6 = 2.08 \times 10^5$ μg/g

Air, Ecology:

Water, Ecology:

Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 1{,}540 = 164.8$ μg/m^3

$EPC_{AH3} = 0.081 \times 1{,}540 = 124.7$ μg/m^3

$EPC_{WH1} = 15 \times 124.7 = 1{,}871$ μg/l

$EPC_{WH2} = 0.4 \times 1{,}540 = 616$ μg/l

$EPC_{LH} = 0.2 \times 616 = 123$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

16A200
CHLORONAPHTHALENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			6.93E4		125		
Water, $\mu g/l$ (ppm Wt)			1.04E6		616		
Land, $\mu g/g$ (ppm Wt)			2.08E5		123		

*To be multiplied by dilution factor

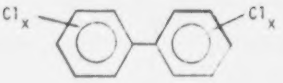
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			125		
Water, $\mu g/l$ (ppm Wt)			616		
Land, $\mu g/g$ (ppm Wt)			123		

CATEGORY: 16A

WLN:

(PCB's) POLYCHLORINATED BIPHENYLS: $C_{12}Cl_n$ (aroclors). 16A220 Depending on the degree of halogenation, polychlorinated biphenyls vary from colorless, oily liquids to black resins.

STRUCTURE:



PROPERTIES:

bp: 278-475; slightly soluble in water; 100 to 1,000 μg/ℓ (ref. 9). The density, boiling point, and melting point increase with chlorine content (ref. 11); soluble in lipids (ref. 11).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Polychlorinated biphenyls are produced by the chlorination of biphenyl. They are remarkably stable and resist attack by water, acids, and bases. They are not easily biodegraded (ref. 9). Biphenyls may have 1 to 10 attached chlorine atoms, making possible over 200 compounds (ref. 9). Concentrations of PCB's ranging from 2.0-2.8 μg/ℓ in the Milwaukee River have been reported; concentration in Lake Michigan is reported as 0.01 μg/ℓ (ref. 11).

It is estimated that 41 to 45 percent of the general population of the United States have PCB levels of 1.0 mg/kg or higher in adipose tissue (ref. 9). PCB's are not believed to be naturally occurring compounds, but are manufactured as mixtures containing specified amounts of chlorine. Such mixtures are referred to by the trademark name Aroclors followed by a four-digit number; the last two digits of the number indicate the percentage of chlorine.

PCB's released to the atmosphere are generally adsorbed to particulate matter. PCB level averaged 3 ng/m^3 for four U.S. cities between 1968 and 1970 (ref. 15).

TOXIC PROPERTIES, HEALTH EFFECTS:

Exposure to PCB's can cause acne, respiratory tract irritation and liver injury (ref. 5). PCB's are considered to be cumulative poisons, and they may be absorbed through the skin (ref. 5). Workers exposed to 0.1 mg/m^3 of the vapors of Aroclor 1242 experienced effects (ref. 5). Animal studies indicate that acute toxicity of the PCB's varies with the specific mixture.

Mixture	LD_{50} (oral, rat) in mg/kg	Mixture	LD_{50} (oral, rat) in mg/kg	Mixture	LD_{50} (oral, rat) in mg/kg
Aroclor 1221	3,980	Aroclor 1254	1,295	Aroclor 1268	10,900
Aroclor 1232	4,470	Aroclor 1260	1,315	Aroclor 2565	6,310
Aroclor 1242	4,250	Aroclor 1262	11,300	Aroclor 4465	16,000
Aroclor 1248	11,000				

Polychlorinated biphenyls have produced carcinogenic responses in rats and mice. The EPA/NIOSH ordering number for PCB's considered collectively is 4212. The lowest dosage to produce a carcinogenic effect is 1,200 mg/kg. The adjusted ordering number is 3.5. Teratogenic effects are also reported (ref. 15).

Aquatic Toxicity: The cumulative potential of PCB's is of great concern in considering toxicity to aquatic life. PCB's at 0.01 μg/ℓ in water have been known to accumulate in fish up to 200,000 times the water concentration. 96-hr TLm's range generally between 1 and 10 μg/ℓ (ref. 11).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV: 0.5 mg/m^3 (for chlorodiphenyls containing 54% chlorine); 1 mg/m^3 for those with 42% chlorine.
PCB's are the subject of a NIOSH criteria document. The recommendation for occupational exposure to PCB's is 1 $\mu g/m^3$ (ref. 13). Polychlorinated biphenyls are on EPA Consent Decree Priority I List.
EPA 1976 water quality criteria: 0.001 μg/ℓ for freshwater and marine aquatic life and for consumers thereof (ref. 11).
NAS/NAE 1972 recommended water quality criteria: 0.002 μg/ℓ for protection of aquatic life. PCB concentrations in whole fish should not exceed 0.5 mg/kg of the wet weight for protection of fish-eating birds and mammals (ref. 9). EPA Toxic Pollutant Effluent Standards: no discharge permitted based on ambient criterion of 0.001 μg/ℓ (ref. 14)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 1 $\mu g/m^3$
Water, Health: 5 x 0.001 = 0.005 μg/ℓ
Land, Health: 0.2 x 0.005 = 0.001 μg/g

Air, Ecology:
Water, Ecology: 5 x 0.001 = 0.005 μg/ℓ
Land, Ecology: 0.2 x 0.005 = 0.001 μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

EPC_{AH1} = 1/420 = 0.0024 $\mu g/m^3$
EPC_{WHS} = 0.001 μg/ℓ
EPC_{LH} = 0.2 x 0.001 = 0.0002 μg/g
EPC_{AC2} = $10^3/(6 \times 3.5)$ = 48 $\mu g/m^3$
EPC_{WC} = 15 x 48 = 714 μg/ℓ
EPC_{LC} = 0.2 x 714 = 143 μg/g

EPC_{WES} = 0.001 μg/ℓ
EPC_{LE} = 0.2 x 0.001 = 0.0002 μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

X
16A220
POLYCHLORINATED BIPHENYLS (PCBs)

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.0E0		0.0024		
Water, $\mu g/l$ (ppm Wt)			5.0E-3	5.0E-3	0.001	0.001	
Land, $\mu g/g$ (ppm Wt)			1.0E-3	1.0E-3	0.0002	0.0002	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			0.0024		48
Water, $\mu g/l$ (ppm Wt)	0.001	0.001			714
Land, $\mu g/g$ (ppm Wt)			0.0002	0.0002	143

REFERENCES: CATEGORY 16A

Halogenated Aromatic Hydrocarbons - Ring Substituted Aromatics

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CATEGORY 16

HALOGENATED AROMATIC COMPOUNDS

SUBCATEGORY: 16B - Aromatics with Halogenated Alkyl Side Chains

Summary of Subcategory

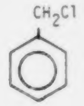
Total number of compounds in subcategory	4
number of parent compounds with subspecies	1
number of subspecies	3
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	1

Consent Decree compounds included in subcategory: None

CATEGORY: 16B **WLN**: G1R

α-CHLOROTOLUENE: C_7H_7Cl (benzyl chloride, (chloromethyl)benzene). **STRUCTURE**:

A colorless liquid with an unpleasant, irritating odor. 16B020



PROPERTIES:

Molecular wt: 126.59; mp: -43; bp: 179.3; d: 1.102_{20}^{20}; vap. d: 4.36; vap. press: 11 mm at 66°; insoluble in water

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

α-Chlorotoluene decomposes when heated in the presence of iron (ref. 1).

The odor threshold in air for α-chlorotoluene is reported as 0.047 ppm or 0.24 mg/m^3 (ref. 2).

TOXIC PROPERTIES, HEALTH EFFECTS:

α-Chlorotoluene is highly irritating to eyes and upper respiratory tract. At 16 ppm (83 mg/m^3) for 1 minute, it is intolerable to man (ref. 3).

LD_{50} (oral, rat): 1,231 mg/kg.

LC_{50} (inhalation, rat): 150 ppm for 2 hours; (mouse): 80 ppm for 2 hours.

α-Chlorotoluene is reported to cause tumors in rats. The EPA/NIOSH ordering number is 4101. The lowest dose to induce an oncogenic response is reported as 2100 mg/kg. The adjusted ordering number is 1.9.

Aquatic toxicity: TLm 96: 10-1 ppm (ref. 4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 5 mg/m^3 (1 ppm).

On Second Priority Chemical List of the Chemical Industry Institute of Toxicology (ref. 5).

Benzyl chloride is the subject of a NIOSH Criteria Document. The NIOSH recommendation for occupational exposure is 5 mg/m^3 (1 ppm) as a time-weighted average (ref. 6).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 5.0×10^3 $\mu g/m^3$ (1 ppm)
Water, Health: $15 \times 5 \times 10^3 = 7.5 \times 10^4$ $\mu g/\ell$
Land, Health: $0.2 \times 7.5 \times 10^4 = 1.5 \times 10^4$ $\mu g/g$

Air, Ecology:
Water, Ecology: $100 \times 1 = 100$ $\mu g/\ell$
Land, Ecology: $0.2 \times 100 = 20$ $\mu g/g$

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 5/420 = 12$ $\mu g/m^3$
$EPC_{AH1a} = 1/420 = 0.002$ ppm
$EPC_{WH1} = 15 \times 12 = 180$ $\mu g/\ell$
$EPC_{WH2} = 13.8 \times 5 = 69$ $\mu g/\ell$
$EPC_{LH} = 0.2 \times 69 = 13.8$ $\mu g/g$
$EPC_{AC2} = 10^3/(6 \times 1.9) = 88$ $\mu g/m^3$
$EPC_{WC} = 15 \times 88 = 1,320$ $\mu g/\ell$
$EPC_{LC} = 0.2 \times 1,320 = 264$ $\mu g/g$

$EPC_{WE1} = 50 \times 1 = 50$ $\mu g/\ell$
$EPC_{LE} = 0.2 \times 50 = 10$ $\mu g/g$

16B020
α-CHLOROTOLUENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			5.0E3		12 (0.002)		
Water, $\mu g/l$ (ppm Wt)			7.5E4	1.0E2	69	50	
Land, $\mu g/g$ (ppm Wt)			1.50E4	2.0E1	14	10	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			12 (0.002)		88
Water, $\mu g/l$ (ppm Wt)			69	50	1,320
Land, $\mu g/g$ (ppm Wt)			14	10	264

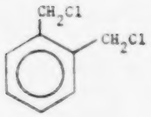
CATEGORY: 16B

WLN:

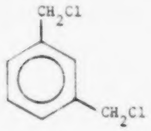
bis(CHLOROMETHYL) BENZENES: $C_6H_4(CH_2Cl)_2$ 16B040

1,2- *bis* (CHLOROMETHYL) BENZENE:	(o-xylene chloride).	16B041
1,3- *bis* (CHLOROMETHYL) BENZENE:	(m-xylene chloride).	16B042
1,4- *bis* (CHLOROMETHYL) BENZENE:	(p-xylene chloride).	16B043

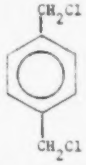
STRUCTURE:



1,2-bis(chloromethyl) benzene



1,3-bis(chloromethyl) benzene



1,4-bis(chloromethyl) benzene

PROPERTIES:

	mol.wt.	mp.	bp.	d.	water solubility
1,2- *bis* (chloromethyl) benzene:	175.07	55	239-41	1.393	insoluble
1,3- *bis* (chloromethyl) benzene:	175.07	34.2	250-5	1.302	insoluble
1,4- *bis* (chloromethyl) benzene:	175.07	100	240-5d	1.417	insoluble

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for bis (chloromethyl) benzenes are not available at this time. However, toxicological characteristics of bis (chloromethyl) benzenes are likely to be similar to those of α-chlorotoluene because of the chemical structure similarity. TLV's for toluene and xylene indicate that toxic potential is not increased by additional substitution on the benzene ring. Data for related compounds are shown below.

Chemical	TLV (mg/m³)	TLV (ppm)	LD_{50} (oral, rat) (mg/kg)	Aquatic toxicity (ppm)
toluene	375	100	5,000	100-10
xylenes(o,m,p)	435	100	5,000	100-10
monochlorobenzene	350	75	2,910	100-1
α-chlorotoluene	5	1	1,231	10-1

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 5 mg/m³ (1 ppm) for α-chlorotoluene.

***MINIMUM ACUTE TOXICITY CONCENTRATIONS:**

Air, Health: 6.9×10^3 μg/m³ (1 ppm)

Water, Health: $15 \times 6.9 \times 10^3 = 1.04 \times 10^5$ μg/l

Land, Health: $0.2 \times 1.04 \times 10^5 = 2.1 \times 10^4$ μg/g

Air, Ecology:

Water, Ecology: $100 \times 1 = 100$ μg/l

Land, Ecology: $0.2 \times 100 = 20$ μg/g

***ESTIMATED PERMISSIBLE CONCENTRATIONS:**

$EPC_{AH1} = 10^3 \times 6.9/420 = 16$ μg/m³

$EPC_{AH1a} = 1/420 = 2.38 \times 10^{-3}$ ppm

$EPC_{WH1} = 15 \times 16 = 240$ μg/l

$EPC_{WH2} = 13.8 \times 6.9 = 95$ μg/l

$EPC_{LH} = 0.2 \times 95 = 19$ μg/g

$EPC_{WE1} = 50 \times 1 = 50$ μg/l

$EPC_{LE} = 0.2 \times 50 = 10$ μg/g

*Based on data for α-chlorotoluene;

$$\text{Molecular wt ratio} = \frac{175.07\ \text{(bis(chloromethyl)benzene)}}{126.59\ (\alpha\text{-chlorotoluene})} = 1.383$$

16B040
bis (CHLOROMETHYL) BENZENES

EMISSION LEVEL GOALS†

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			6.9E3 (1.0)		16 (0.002)		
Water, $\mu g/l$ (ppm Wt)			1.04E5	1.0E2	95	50	
Land, $\mu g/g$ (ppm Wt)			2.1E4	2.0E1	19	10	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS †

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			17 (2.38×10^{-3})		
Water, $\mu g/l$ (ppm Wt)			99	50	
Land, $\mu g/g$ (ppm Wt)			20	10	

† Based on data for α-chlorotoluene.

REFERENCES: CATEGORY 16B

Halogenated Aromatic Hydrocarbons - Aromatics with Halogenated Alkyl Side Chains

1. Windholz, M., Ed. The Merck Index: An Encyclopedia of Chemicals and Drugs, Ninth Edition. Merck & Co., Inc., Rahway, NJ (1976).

2. Billings, C. E. Technological Sources of Air Pollution. Industrial Pollution, N. I. Sax, Ed., Van Nostrand Rheinhold Co., New York, NY (1974).

3. American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values for Substances in Workroom Air with Supplements, Third Edition. American Conference of Governmental Industrial Hygienists, Cincinnati, OH (1974).

4. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

5. Chemical Industry Institute of Toxicology. Second Priority List. Chemical Industry Institute of Toxicology: Annual Report. Research Triangle Park, NC (1976).

6. National Institute for Occupational Safety and Health. Criteria for a Recommended Standard: Occupational Exposure to Benzyl Chloride. National Institute for Occupational Safety and Health. U.S. Department of Health, Education, and Welfare, DHEW (NIOSH) Publication No. 78-182 (1978).

CATEGORY 17

AROMATIC NITRO COMPOUNDS

SUBCATEGORY: 17A - Simple Aromatic Nitro Compounds

Summary of Subcategory

Total number of compounds in subcategory	11
number of parent compounds with subspecies	2
number of subspecies	9
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	1

Consent Decree compounds included in subcategory: 7

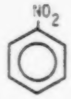
17A020	Nitrobenzene
17A081	2,6-Dinitrotoluene
17A082	3,4-Dinitrotoluene
17A083	2,3-Dinitrotoluene
17A084	2,4-Dinitrotoluene
17A085	2,5-Dinitrotoluene
17A086	3,5-Dinitrotoluene

CATEGORY: 17A

WLN: WNR

NITROBENZENE: $C_6H_5NO_2$. 17A020

STRUCTURE:



A colorless to pale yellow, oily liquid or bright yellow crystals with odor similar to volatile oil of almonds.

PROPERTIES:

Molecular wt: 123.11; mp: 6; bp: 210-11; d: 1205; vap. press: 1 mm at 44.4; vap. d: 4.25; soluble in about 500 parts water; volatile with steam.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

All nitro compounds are potentially explosive.

The odor threshold in air for nitrobenzene is 0.0047 ppm or 23 $\mu g/m^3$ (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

Nitrobenzene is toxic by ingestion and by inhalation. It is readily absorbed through the skin. Effects of exposure include cyanosis, methemoglobinemia, and central nervous system effects (ref. 2).

A woman is reported to have experienced blood effects as a result of ingesting 200 mg/kg of nitrobenzene (ref. 3).

LD_{Lo} (oral, dog): 750 mg/kg.

LD_{Lo} (oral, rabbit): 700 mg/kg.

Aquatic toxicity: TLm 96: 100-10 ppm.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Nitrobenzene is on EPA Consent Decree Priority III List.

TLV = 5 mg/m^3 (1 ppm) skin.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 5.0×10^3 $\mu g/m^3$ (1 ppm)
Water, Health: $15 \times 5.0 \times 10^3 = 7.5 \times 10^4$ $\mu g/\ell$
Land, Health: $0.2 \times 7.5 \times 10^4 = 1.5 \times 10^4$ $\mu g/g$

Air, Ecology:
Water, Ecology: $100 \times 10 = 1.0 \times 10^3$ $\mu g/\ell$
Land, Ecology: $0.2 \times 1.0 \times 10^3 = 200$ $\mu g/g$

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 5/420 = 12$ $\mu g/m^3$
$EPC_{AH1a} = 1/420 = 0.002$ ppm
$EPC_{WH1} = 15 \times 12 = 180$ $\mu g/\ell$
$EPC_{WH2} = 13.8 \times 5 = 69$ $\mu g/\ell$
$EPC_{LH} = 0.2 \times 69 = 14$ $\mu g/g$

$EPC_{WE1} = 50 \times 10 = 500$ $\mu g/\ell$
$EPC_{LE} = 0.2 \times 500 = 100$ $\mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

17A020
NITROBENZENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			5.0E3 (1)		12 (0.002)		
Water, $\mu g/l$ (ppm Wt)			7.5E4	1.0E3	69	500	
Land, $\mu g/g$ (ppm Wt)			1.5E4	2.0E2	14	100	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			12 (0.002)		
Water, $\mu g/l$ (ppm Wt)			69	500	
Land, $\mu g/g$ (ppm Wt)			14	100	

CATEGORY: 17A

WLN: WNR B; WNR C; WNR D

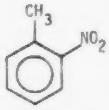
NITROTOLUENES: $C_7H_7NO_2$ (methylnitrobenzenes). 17A040

2-NITROTOLUENE: yellow liquid. 17A041

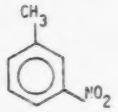
3-NITROTOLUENE: liquid. 17A042

4-NITROTOLUENE: yellowish crystals. 17A043

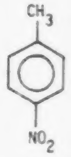
STRUCTURE:



2-Nitrotoluene
(o-nitrotoluene)



3-Nitrotoluene
(m-nitrotoluene)



4-Nitrotoluene
(p-nitrotoluene)

PROPERTIES:	Mol. wt.	mp	bp	d_4^{20}	Water Solubility	vap. d	vap. press.
2-nitrotoluene	137.13	-10	222	1.163	insoluble	4.72	1 mm at 50°
3-nitrotoluene	137.13	15.5	231.9	1.157	0.5 g/ℓ water	4.72	1 mm at 50.2°
4-nitrotoluene	137.13	53-54	238	1.286	insoluble	4.72	1 mm at 53.7°

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

All nitro compounds are potentially explosive.

TOXIC PROPERTIES, HEALTH EFFECTS:

The nitrotoluenes are low-grade methemoglobin formers; cases of poisoning are uncommon. They are significantly less toxic than nitrobenzene; however, the different isomers exhibit different levels of toxicity (ref. 4). They can be absorbed through the intact skin and the respiratory tract (ref. 5).

	LD_{50} (oral, rat)	Aquatic toxicity
2-nitrotoluene	891 mg/kg	TLm 96: 100-10 ppm
3-nitrotoluene	1,072 mg/kg	——
4-nitrotoluene	2,144 mg/kg	——

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 30 mg/m^3 (5 ppm).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 3.0×10^4 μg/m^3 (5 ppm)

Water, Health: $15 \times 3.0 \times 10^4 = 4.5 \times 10^5$ μg/ℓ

Land, Health: $0.2 \times 4.5 \times 10^5 = 9.0 \times 10^4$ μg/g

Air, Ecology:

Water, Ecology: $100 \times 10 = 1.0 \times 10^3$ μg/ℓ

Land, Ecology: $0.2 \times 1.0 \times 10^3 = 200$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 30/420 = 71$ μg/m^3

$EPC_{AH1a} = 5/420 = 0.01$ ppm

$EPC_{WH1} = 15 \times 71 = 1{,}065$ μg/ℓ

$EPC_{WH2} = 13.8 \times 30 = 414$ μg/ℓ

$EPC_{LH} = 0.2 \times 414 = 83$ μg/g

$EPC_{WE1} = 50 \times 10 = 500$ μg/ℓ

$EPC_{LE} = 0.2 \times 500 = 100$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

17A040
NITROTOLUENES

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			3.0E4 (5)		71 (0.01)		
Water, $\mu g/l$ (ppm Wt)			4.5E5	1.0E3	414	500	
Land, $\mu g/g$ (ppm Wt)			9.0E4	2.0E2	83	100	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

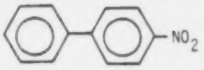
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			71 (0.01)		
Water, $\mu g/l$ (ppm Wt)			414	500	
Land, $\mu g/g$ (ppm Wt)			83	100	

CATEGORY: 17A

WLN: WNR DR

4-NITROBIPHENYL: $C_{12}H_9NO_2$ (p-nitrobiphenyl, 4-nitrodiphenyl). Crystallizes as yellow needles from ethanol. 17A060

STRUCTURE:



PROPERTIES:

Molecular wt: 199.21; mp: 114-114.5; bp: 340 at 760 mm; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

4-Nitrobiphenyl is reduced in the presence of activated iron to the corresponding amine.

All nitro compounds are potentially explosive.

There is evidence that 4-nitrobiphenyl is metabolized in vivo to 4-aminobiphenyl, a highly carcinogenic aromatic amine (ref. 6).

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{50} (oral, rat): 2,230 mg/kg.

4-Nitrobiphenyl is recognized as one of the more potent human bladder carcinogens (ref. 4). Human bladder cancer has been linked with occupational exposure. In high concentrations (5,500 mg/kg), the compound has produced bladder cancer in dogs (refs. 3,7). The EPA/NIOSH ordering number for 4-nitrobiphenyl is 7212. Considering carcinogenic potential of 4-nitrobiphenyl together with that of its metabolite, 4-aminodiphenyl, the EPA/NIOSH ordering number is 7526, and the lowest dosage resulting in an oncogenic response is 140 mg/kg. The adjusted ordering number for the compounds considered collectively is 54.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

4-Nitrobiphenyl is classified by ACGIH as a human carcinogen. No TLV has been assigned; because of the high incidence of cancer, no exposure by any route should be permitted.

4-Nitrobiphenyl is the subject of a NIOSH Hazard Review Document (ref. 7).

4-Nitrobiphenyl is designated by OSHA as a cancer suspect agent; special precautions for exposed workers are prescribed (ref. 8).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/54 = 1.3 \times 10^3\ \mu g/m^3$ Air, Ecology:
Water, Health: $15 \times 1.3 \times 10^3 = 2.0 \times 10^4\ \mu g/\ell$ Water, Ecology:
Land, Health: $0.2 \times 2.0 \times 10^4 = 4.0 \times 10^3\ \mu g/g$ Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 2,230 = 239\ \mu g/m^3$
$EPC_{AH3} = 0.081 \times 2,230 = 180\ \mu g/m^3$
$EPC_{WH1} = 15 \times 180 = 2,700\ \mu g/\ell$
$EPC_{WH2} = 0.4 \times 2,230 = 890\ \mu g/\ell$
$EPC_{LH} = 0.2 \times 890 = 178\ \mu g/g$
$EPC_{AC2} = 10^3/(6 \times 54) = 3\ \mu g/m^3$
$EPC_{WC} = 15 \times 3 = 45\ \mu g/\ell$
$EPC_{LC} = 0.2 \times 45 = 9\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

X
17A060
4-NITROBIPHENYL

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.3E3		3		
Water, $\mu g/l$ (ppm Wt)			2.0E4		45		
Land, $\mu g/g$ (ppm Wt)			4.0E3		9		

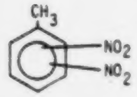
*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			180		3
Water, $\mu g/l$ (ppm Wt)			890		45
Land, $\mu g/g$ (ppm Wt)			178		9

CATEGORY: 17A

WLN:

STRUCTURE:



DINITROTOLUENES: $C_7H_6N_2O_4$. 17A080

Dinitrotoluenes crystallize mainly in the form of yellow needles from ethanol or carbon disulfide.

2,6-DINITROTOLUENE: 17A081
3,4-DINITROTOLUENE: 17A082
2,3-DINITROTOLUENE: 17A083
2,4-DINITROTOLUENE: 17A084
2,5-DINITROTOLUENE: 17A085
3,5-DINITROTOLUENE: 17A086

PROPERTIES:	Mol. wt.	mp	bp	d	solubility	vap. d.
2,6-Dinitrotoluene	182.14	66	--	1.283		
3,4-Dinitrotoluene	182.14	58.3	--	1.259	insoluble	
All isomers	182.14	52-93	sublimes to 300°C	1.259-1.321	insoluble to slightly soluble	6.27 (for 2,4 isomer)

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

All nitro compounds are potentially explosive.

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxic effects of dinitrotoluenes are similar to those of other aromatic nitro compounds. It causes central nervous system and blood disorders (ref. 4).

Dinitrotoluenes may be absorbed through the skin.

	LD_{50} (oral, rat)	Aquatic toxicity
2,3-dinitrotoluene	1,122 mg/kg	TLm 96: 100-10 ppm
2,4-dinitrotoluene	268 mg/kg	TLm 96: 100-10 ppm
2,5-dinitrotoluene	707 mg/kg	TLm 96: 100-10 ppm
2,6-dinitrotoluene	177 mg/kg	TLm 96: 100-10 ppm
3,4-dinitrotoluene	177 mg/kg	TLm 96: 100-10 ppm
3,5-dinitrotoluene		

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Dinitrotoluenes are on EPA Consent Decree Priority III List.

TLV = 1.5 mg/m^3 (By analogy with limits recommended for nitro and dinitro-benzenes).

On First Priority Chemicals List of the Chemical Industry Institute of Toxicology (ref.10).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 1.5×10^3 μg/m^3
Water, Health: $15 \times 1.5 \times 10^3 = 2.25 \times 10^4$ μg/ℓ
Land, Health: $0.2 \times 2.25 \times 10^4 = 4.5 \times 10^3$ μg/g

Air, Ecology:
Water, Ecology: $100 \times 10 = 1.0 \times 10^3$ μg/ℓ
Land, Ecology: $0.2 \times 1.0 \times 10^3 = 200$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 1.5/420 = 3.6$ μg/m^3
$EPC_{WH1} = 15 \times 3.6 = 54$ μg/ℓ
$EPC_{WH2} = 13.8 \times 1.5 = 21$ μg/ℓ
$EPC_{LH} = 0.2 \times 21 = 4$ μg/g

$EPC_{WE1} = 50 \times 10 = 500$ μg/ℓ
$EPC_{LE} = 0.2 \times 500 = 100$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

X
17A080
DINITROTOLUENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.5E3		3.6		
Water, $\mu g/l$ (ppm Wt)			2.25E4	1.0E3	21	500	
Land, $\mu g/g$ (ppm Wt)			4.5E3	2.0E2	4	100	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			3.6		
Water, $\mu g/l$ (ppm Wt)			21	500	
Land, $\mu g/g$ (ppm Wt)			4	100	

REFERENCES: CATEGORY 17A

Aromatic Nitro Compounds - Simple Aromatic Nitro Compounds

1. Billings, C. E. Technological Sources of Air Pollution. *Industrial Pollution*, N. I. Sax, Ed., Van Nostrand Rheinhold Co., New York, NY (1974).

2. Windholz, M., Ed. The Merck Index: An Encyclopedia of Chemicals and Drugs, Ninth Edition. Merck & Co., Inc., Rahway, NJ (1976).

3. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, M for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

4. American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values for Substances in Workroom Air with Supplements, Third Edition. American Conference of Governmental Industrial Hygienists, Cincinnati, OH (1974).

5. Hamblin, D. O. Aromatic Nitro and Amino Compounds. *Industrial Hygiene and Toxicology*, *Second Revised Edition*, *Vol. 2*, F. A. Patty, Ed., Interscience Publishers, New York, NY (1963).

6. International Agency for Research on Cancer. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Man, Vol. 4, Lyon, France. A World Health Organization (WHO), Geneva (1974).

7. Occupational Safety and Health Administration, Department of Labor. Hazard Review Document. Federal Register 39, No. 20, 3756-3757 (1974).

8. U.S. Department of Labor. Occupational Safety and Health Standards. Toxic and Hazardous Substances. Title 29 Code Federal Regulations, Part 1910.

9. Sax, N. I., Ed. Dangerous Properties of Industrial Materials, Fourth Edition. Van Nostrand Reinhold Co., New York, NY (1975).

10. Chemical Industry Institute of Toxicology. Second Priority List. Chemical Industry Institute of Toxicology: Annual Report. Research Triangle Park, NC (1976).

CATEGORY 17

AROMATIC NITRO COMPOUNDS

SUBCATEGORY: 17B - Aromatic Nitro Compounds with Other Functional Groups

Summary of Subcategory

Total number of compounds in subcategory	5
number of parent compounds with subspecies	1
number of subspecies	3
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

Consent Decree compounds included in subcategory: 5

17B021	1-Methoxy-2-nitrobenzene
17B022	1-Methoxy-3-nitrobenzene
17B023	1-Methoxy-4-nitrobenzene
17B040	1-Chloro-2-nitrobenzene
17B060	1-Chloro-4-nitrobenzene

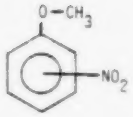
CATEGORY: 17B

WLN:

METHOXYNITROBENZENES: $C_7H_7NO_3$ (nitroanisoles, nitrophenyl methyl ethers). 17B020

1-METHOXY-2-NITROBENZENE: Colorless to yellowish liquid. 17B021
1-METHOXY-3-NITROBENZENE: Crystals. 17B022
1-METHOXY-4-NITROBENZENE: Crystals. 17B023

STRUCTURE:



PROPERTIES:

	mol. wt.	mp.	bp.	d:	solubility in water
1-methoxy-2-nitrobenzene	153.1	10.45	276.8^{757}	1.2540^{20}	insoluble
1-methoxy-3-nitrobenzene	153.1	38.9	258	1.373^{18}	insoluble
1-methoxy-4-nitrobenzene	153.1	54	274	1.219^{60}_{4}	insoluble

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Methoxynitrobenzenes are used as intermediates in dye synthesis and in general organic synthesis (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{50} (oral, mammal): 4,700 mg/kg for 1-methoxy-4-nitrobenzene (ref. 2).

Aryl-substituted anisoles such as 1-methoxy-3-nitrobenzene and 1-methoxy-4-nitrobenzene are reported to be demethylated to form the phenols, which are excreted largely as the glucuronates and ethereal sulfates (ref. 3).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Nitrobenzenes are on the EPA Consent Decree List, Priority 3.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$45 \times 4{,}700 = 2.12 \times 10^5$ μg/m^3	Air, Ecology:	
Water, Health:	$15 \times 2.12 \times 10^5 = 3.18 \times 10^6$ μg/l	Water, Ecology:	
Land, Health:	$0.2 \times 3.18 \times 10^6 = 6.4 \times 10^5$ μg/g	Land, Ecology:	

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 4{,}700 = 503$ μg/m^3

$EPC_{AH3} = 0.081 \times 4{,}700 = 381$ μg/m^3

$EPC_{WH1} = 15 \times 381 = 5{,}715$ μg/l

$EPC_{WH2} = 0.4 \times 4{,}700 = 1{,}880$ μg/l

$EPC_{LH} = 0.2 \times 1{,}880 = 376$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

17B020
METHOXYNITROBENZENES

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.12E5		381		
Water, $\mu g/l$ (ppm Wt)			3.18E6		1,880		
Land, $\mu g/g$ (ppm Wt)			6.4E5		376		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

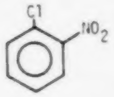
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			381		
Water, $\mu g/l$ (ppm Wt)			1,880		
Land, $\mu g/g$ (ppm Wt)			376		

CATEGORY: 17B

WLN: WNR BG

1-CHLORO-2-NITROBENZENE: $C_6H_4NO_2Cl$ (o-chloronitrobenzene).
Yellow crystals. 17B040

STRUCTURE:



PROPERTIES:

Molecular wt: 157.6; mp: 32-33; bp: 245-246; d: 1.305; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

All nitro compounds are potentially explosive.

TOXIC PROPERTIES, HEALTH EFFECTS:

Intoxication from 1-chloro-2-nitrobenzene may be serious. It can cause poisoning by the pulmonary route, and its effects are cumulative. Cyanosis and blood changes also occur. Acute toxicity is more severe than for 1-chloro-4-nitrobenzene (ref. 4).

LD_{50} (oral, rat): 288 mg/kg.

Aquatic toxicity: TLm 96: 1,000-100 ppm.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Chlorobenzenes and nitrobenzenes are on the EPA Consent Decree List, Priorities 2 and 3, respectively. TLV for 1-chloro-4-nitrobenzene is 1 mg/m^3 (0.16 ppm).

***MINIMUM ACUTE TOXICITY CONCENTRATIONS**:

Air, Health: 1.0×10^3 $\mu g/m^3$ (0.16 ppm)

Water, Health: $15 \times 1.0 \times 10^3 = 1.5 \times 10^4$ $\mu g/l$

Land, Health: $0.2 \times 1.5 \times 10^4 = 3.0 \times 10^3$ $\mu g/g$

Air, Ecology:

Water, Ecology: $100 \times 100 = 1.0 \times 10^4$ $\mu g/l$

Land, Ecology: $0.2 \times 1.0 \times 10^4 = 2.0 \times 10^3$ $\mu g/g$

***ESTIMATED PERMISSIBLE CONCENTRATIONS**:

$EPC_{AH1} = 10^3 \times 1/420 = 2.38$ $\mu g/m^3$

$EPC_{AH1a} = 0.16/420 = 3.8 \times 10^{-4}$ ppm

$EPC_{WH1} = 15 \times 2.38 = 35.7$ $\mu g/l$

$EPC_{WH2} = 13.8 \times 1 = 13.8$ $\mu g/l$

$EPC_{LH} = 0.2 \times 13.8 = 2.76$ $\mu g/g$

$EPC_{WE1} = 50 \times 100 = 5,000$ $\mu g/l$

$EPC_{LE} = 0.2 \times 5,000 = 1.0 \times 10^3$ $\mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

X
17B040
1-CHLORO-2-NITROBENZENE

EMISSION LEVEL GOALS †

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.0E3 (0.16)		2.4 (0.0004)		
Water, µg/l (ppm Wt)			1.5E4	1.0E4	14	5,000	
Land, µg/g (ppm Wt)			3.0E3	2.0E3	3	1,000	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS †

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			2.4 (0.0004)		
Water, µg/l (ppm Wt)			14	5,000	
Land, µg/g (ppm Wt)			3	1,000	

†Health values based on TLV for 1-chloro-4-nitrobenzene.

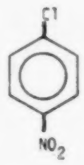
CATEGORY: 17B

1-CHLORO-4-NITROBENZENE: $C_6H_4NO_2Cl$ (p-chloronitrobenzene, p-nitrochlorobenzene). 17B060

A yellowish crystal.

WLN: WNR DG

STRUCTURE:



PROPERTIES:

Molecular wt: 157.56; mp: 83.6; bp: 242^{760}; d: 1.2979; vap.d: 5.43; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

1-Chloro-4-nitrobenzene can be formed from chlorobenzene and fuming HNO_3 (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

1-Chloro-4-nitrobenzene is a CNS depressant and a sensitizer (ref. 5). When heated it emits toxic fumes of NO_x and chlorides (ref. 4). Like nitrobenzene, 1-chloro-4-nitrobenzene may be absorbed through the skin as well as through the lungs and gives rise to methemoglobin. Cyanoses, headache, and weakness result from exposure (ref. 6).

LD_{50} (oral, mouse): 1,414 mg/kg

Aquatic toxicity: Aquatic toxicity is likely to be similar to that of 1-chloro-2-nitrobenzene.

TLm 96: 1,000-100 ppm for 1-chloro-2-nitrobenzene.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 1 mg/m^3 (0.16 ppm)

Chlorobenzenes and nitrobenzenes are on the EPA Consent Decree List, Priorities 2 and 3, respectively.

* MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 1.0×10^3 $\mu g/m^3$ (0.16 ppm)

Air, Ecology:

Water, Health: $15 \times 1.0 \times 10^3 = 1.5 \times 10^4$ $\mu g/l$

Water, Ecology: $100 \times 100 = 1.0 \times 10^4$ $\mu g/l$

Land, Health: $0.2 \times 1.5 \times 10^4 = 3.0 \times 10^3$ $\mu g/g$

Land, Ecology: $0.2 \times 1.0 \times 10^4 = 2.0 \times 10^3$ $\mu g/g$

* ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 1/420 = 2.38\ \mu g/m^3$

$EPC_{AH1a} = 0.16/420 = 3.8 \times 10^{-4}$ ppm

$EPC_{WH1} = 15 \times 2.38 = 35.7\ \mu g/l$

$EPC_{WE1} = 50 \times 100 = 5{,}000\ \mu g/l$

$EPC_{WH2} = 13.8 \times 1 = 13.8\ \mu g/l$

$EPC_{LH} = 0.2 \times 13.8 = 2.76\ \mu g/g$

$EPC_{LE} = 0.2 \times 5{,}000 = 1.0 \times 10^3\ \mu g/g$

* Ecology values based on TLm-96 for 1-chloro-2-nitrobenzene.

MULTIMEDIA ENVIRONMENTAL GOALS

X
17B060
1-CHLORO-4-NITROBENZENE

EMISSION LEVEL GOALS	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.0E3 (0.16)		2.4 (0.0004)		
Water, $\mu g/l$ (ppm Wt)			1.5E4	1.0E4	14	5,000	
Land, $\mu g/g$ (ppm Wt)			3.0E3	2.0E3	3	1,000	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			2.4 (0.0004)		
Water, $\mu g/l$ (ppm Wt)			14	5,000	
Land, $\mu g/g$ (ppm Wt)			3	1,000	

REFERENCES: CATEGORY 17B

Aromatic Nitro Compounds - Aromatic Nitro Compounds with Other Functional Groups

1. Windholz, M., Ed. The Merck Index: An Encyclopedia of Chemicals and Drugs, Ninth Edition. Merck & Co., Inc., Rahway, NJ (1976).
2. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).
3. Hake, C. L., and V. K. Rowe. Ethers. Industrial Hygiene and Toxicology, Second Revised Edition, Vol. 2. F. A. Patty, Ed., Interscience Publishers, New York, NY (1963).
4. Sax, N. I., Ed. Dangerous Properties of Industrial Materials, Fourth Edition. Van Nostrand Reinhold Co., New York, NY (1975).
5. Plunkett, E. R. Handbook of Industrial Toxicology, Second Edition, Chemical Publishing Company, Inc., New York (1976).
6. American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values for Substances in Workroom Air with Supplements, Third Edition. American Conference of Governmental Industrial Hygienists, Cincinnati, OH (1974).

CATEGORY 18

PHENOLS

SUBCATEGORY: 18A - Monohydrics

Summary of Subcategory

Total number of compounds in subcategory	24
number of parent compounds with subspecies	6
number of subspecies	21
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	1

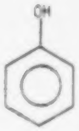
Consent Decree compounds included in subcategory: 2

18A020	Phenol
18A142	2,4-Xylenol

CATEGORY: 18A

WLN: QR

STRUCTURE:



PHENOL: C_6H_6O (carbolic acid, hydroxybenzene, oxybenzene, phenic acid, phenylic acid, phenyl hydroxide). 18A020
Colorless needles, characteristic odor; reddens on exposure to air and light.

PROPERTIES:

Molecular wt: 94.11; mp: 43; bp: 181.75; d: 1.072 at 20°/4°; vap. press.: 1 mm at 40.1°C; vap. d: 3.24; soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

The odor threshold for phenol is reported as 0.047 ppm or 180 μg/m^3 (ref. 1). Because of its low volatility, however, phenol is primarily of concern as a water contaminant rather than an air contaminant.

Phenol is obtained from coal tar (refs. 2,3).

If phenolic compounds are present in waters that are chlorinated for disinfection, chlorophenols may be formed (ref. 4).

TOXIC PROPERTIES, HEALTH EFFECTS:

Phenol is absorbed through the gastrointestinal and respiratory tracts and through the skin. Acute and chronic poisoning may result from exposure. Chronic poisoning results in damage to the liver and kidney (ref. 5). Human ingestion of 14 mg/kg has resulted in gastrointestinal effects, and ingestion of 140 mg/kg is reported to cause death to a human (ref. 6).

LD_{50} (oral, rat): 414 mg/kg.

Phenol is reported to produce tumors in mice. The EPA/NIOSH ordering number is 3,121. The lowest effective dosage is 4,000 mg/kg; the adjusted ordering number is 0.78. There is no specific evidence of human cancer attributable to phenol (ref. 3).

Experiments with Drosophilia have shown phenol to be highly mutagenic (ref. 7).

Aquatic toxicity: TLm 96: 100-10 ppm. As low as 79 μg/ℓ are toxic to minnows in freshwater after 30 minutes (ref. 4). Concentrations of 1 to 10 mg/ℓ in water result in tainting of fish flesh (ref. 4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 19 mg/m^3 (5 ppm). On EPA Consent Decree Priority III list. On First Priority Chemicals List of the Chemical Industry Institute of Toxicology (ref. 8).

Phenol is the subject of a NIOSH criteria document. NIOSH recommends exposure to phenol vapor, solid, or mists be limited to 20 mg/m^3 as a time-weighted average for up to a 10-hour workday (ref. 9).

EPA 1976 Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 10).

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (for phenols) (ref. 4).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/ℓ (for phenols) (ref. 11).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 1.9×10^4 μg/m^3 (5 ppm)
Water, Health: $5 \times 1 = 5$ μg/ℓ
Land, Health: $0.2 \times 5 = 1.0$ μg/g

Air, Ecology:
Water, Ecology: $100 \times 5 = 500$ μg/ℓ
Land, Ecology: $0.2 \times 500 = 100$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 19/420 = 45$ μg/ℓ
$EPC_{AH1a} = 5/420 = 0.01$ ppm
$EPC_{WH1} = 15 \times 45 = 675$ μg/ℓ
$EPC_{WH2} = 13.8 \times 19 = 260$ μg/ℓ
$EPC_{WHS} = 1$ μg/ℓ (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = .2$ μg/g

$EPC_{WE1} = 50 \times 10 = 500$ μg/ℓ
$EPC_{WE2} = 1,000$ μg/ℓ (to prevent tainting)
$EPC_{WES} = 100$ μg/ℓ (phenolic compounds)
$EPC_{LE} = 0.2 \times 100 = 20$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

18A020
PHENOL

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal[*]		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background[*]
Air, $\mu g/m^3$ (ppm Vol)			1.9E4 (5)		45 (0.01)		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1	100	
Land, $\mu g/g$ (ppm Wt)			1.0E 0	1.0E2	0.2	20	

[*] To be multiplied by dilution factor

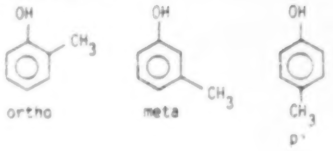
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			45 (0.01)		
Water, $\mu g/l$ (ppm Wt)	1[†]	100[†]	260	500	
Land, $\mu g/g$ (ppm Wt)			0.2	20	

[†] Phenolic compounds.

CATEGORY: 18A

WLN:

STRUCTURE:



18A040

CRESOLS: C_7H_8O (cresylic acid, methylphenol, hydroxytoluene).

m- CRESOL: colorless or yellowish liquid, phenolic odor. 18A041

o- CRESOL: crystals or liquid, phenolic odor. 18A042

p- CRESOL: crystals, phenolic odor. 18A043

PROPERTIES:

Molecular wt: 108.37; density$^{4}_{20}$: 1.034-1.047;
vap. d: 3.72; soluble in water.

	mp	bp	vap. press.
m-cresol	11	202	0.153 mm at 25°C
o-cresol	30	191	0.245 mm at 25°C
p-cresol	35.5	201.8	0.108 mm at 25°C

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Cresols are methyl-substituted hydroxy benzene compounds, i.e., methyl phenols. Ortho, meta and para compounds occur. The meta isomer predominates in mixtures (ref. 2).

Odor recognition level for cresols ranges from 0.9 to 1.21 mg/m^3 or 0.20 to 0.27 ppm (ref. 12). The odor threshold in air for p-cresol is reported as 0.001 ppm or 4 μg/m^3 (ref. 1). Threshold limit for the detection of odor in aqueous solution is reported as 0.00025 mg/ℓ (ref. 3).

Cresols are obtained from coal tar (ref. 2). Due to the low vapor pressure and disagreeable odor, cresols usually do not present an acute inhalation hazard (ref. 3).

Cresols are highly resistant to biological oxidation (ref. 13).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxic properties of cresols are similar to those of phenol. Cresols may be absorbed through the skin. Respiratory hazard is low because of low volatility. Absorption may cause damage to liver, kidney and nervous system (ref. 5). Order of toxicity beginning with most toxic is reported to be as follows: p-cresol; o-cresol; phenol; m-cresol (ref. 14).

	LD_{50} (oral, rat)
m-cresol	242 mg/kg
o-cresol	121 mg/kg
p-cresol	207 mg/kg

Toxicity to aquatic life: tainting of fish may result from concentrations of 0.07 mg/ℓ of mixed cresol isomers (ref. 4). The toxic concentration of p-cresol is 5 ppm for rainbow trout (ref. 15). The 96-hour LC_{50} for p-cresol is reported as 19 mg/ℓ (ref. 16). For mixed cresol isomers, the 96-hour TLm is reported as 10-1 ppm (ref. 6).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV for cresol (all isomers): 22 mg/m^3 (5 ppm). Cresol is the subject of a NIOSH Criteria Document. The NIOSH recommendation for occupational exposure is 10 mg/m^3 (ref. 20).

EPA 1976 Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 10).

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (for phenols) (ref. 4).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/ℓ (for phenols)(ref. 11).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 1.0×10^4 μg/m^3 (2 ppm)
Water, Health: $5 \times 1 = 5$ μg/ℓ
Land, Health: $0.2 \times 5 = 1$ μg/g

Air, Ecology:
Water, Ecology: $100 \times 5 = 500$ μg/ℓ
Land, Ecology: $0.2 \times 500 = 100$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 10/420 = 24$ μg/m^3
$EPC_{AH1a} = 2/420 = 0.005$ ppm
$EPC_{WH1} = 15 \times 24 = 360$ μg/ℓ
$EPC_{WH2} = 13.8 \times 10 = 138$ μg/ℓ
$EPC_{WHS} = 1$ μg/ℓ (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g

$EPC_{WE1} = 50 \times 1 = 50$ μg/ℓ
$EPC_{WE2} = 70$ μg/ℓ (to prevent tainting)
$EPC_{WES} = 100$ μg/ℓ (phenolic compounds)
$EPC_{LE} = 0.2 \times 50 = 10$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

X
18A040
CRESOLS

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)			1.0E4 (2)		24 (0.005)		
Water, μg/l (ppm Wt)			5.0E0	5.0E2	1	50	
Land, μg/g (ppm Wt)			1.0E 0	1.0E2	0.2	10	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)			24 (0.005)		
Water, μg/l (ppm Wt)	1 †	100 †	138	50	
Land, μg/g (ppm Wt)			0.2	10	

† Phenolic compounds.

166<

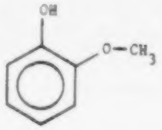
CATEGORY: 18A

2-METHOXYPHENOL: $C_7H_8O_2$ (2-hydroxy anisole, guaiacol, 1-hydroxy-2-methoxybenzene, methylcatechol). 18A060

A clear, pale yellow liquid or solid, with a mild aromatic odor.

WLN: QR BO1

STRUCTURE:



PROPERTIES:

Molecular wt: 124.15; mp: 32; bp: 205.05^{760}; d: 1.1287; vap.d: 4.27; vap.p: 100 mm at 144°; slightly soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Methoxyphenols have been identified in samples taken from river water and from finished drinking water (ref. 17). It is formed from the destructive distillation of hardwoods (ref. 18).

Uses of 2-methoxyphenol include antioxidant, antigumming agent in hydrocarbon solvents, oxidation control in printing ink, and chemical intermediate. It also has antiseptic properties. and has been used medically as an expectorant and antipyretic agent (ref. 18).

Methoxyphenol in air can be trapped by passing the sample through an organic solvent or through sodium hydroxide for collection. Vapor phase or paper chromatography and mass spectrometry are used for specific circumstances (ref. 18).

TOXIC PROPERTIES, HEALTH EFFECTS:

2-Methoxyphenol is reported to be about one-third as toxic as phenol and to have pharmacological properties quite similar to phenol. Medical experience indicates that toxic quantities can be absorbed through the skin quite readily. It is severely injurious to the eyes. It is not likely that vapor inhalation would constitute a serious hazard. In general, the material may be more hazardous to human beings than to lower animals. In one case, a 9-yr old girl died after swallowing 5 ml (ref. 18).

LD_{50} (oral, rat): 725 mg/kg (ref. 2).

Aquatic toxicity: 2-methoxyphenol is reported to cause tainting of fish flesh at a level of 0.082 mg/ℓ (ref. 4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 µg/l of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 10).

NAS/NAE 1972 Water Quality Criteria: 1 µg/l of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 µg/l at any time or place; application factor of 0.05 (ref. 4).

U.S. Public Health Service Drinking Water Standards, 1962--Levels for alternate source selection: 1 µg/l (ref. 11).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 725 = 3.26 \times 10^4$ µg/m^3

Water, Health: $5 \times 1 = 5$ µg/l

Land, Health: $0.2 \times 5 = 1$ µg/g

Air, Ecology:

Water, Ecology: $100 \times 5 = 500$ µg/l

Land, Ecology: $0.2 \times 500 = 100$ µg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 725 = 77.6$ µg/m^3

$EPC_{AH3} = 0.081 \times 725 = 58.7$ µg/m^3

$EPC_{WH1} = 15 \times 58.7 = 881$ µg/l

$EPC_{WH2} = 0.4 \times 725 = 290$ µg/l

$EPC_{WHS} = 1$ µg/l (phenolic compounds)

$EPC_{LH} = 0.2 \times 1 = 0.2$ µg/g

$EPC_{WE2} = 82$ µg/l (to prevent tainting)

$EPC_{WES} = 100$ µg/l (phenolic compounds)

$EPC_{LE} = 0.2 \times 82 = 16.4$ µg/g

MULTIMEDIA ENVIRONMENTAL GOALS

18A060
2-METHOXYPHENOL

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			3.26E4		58.7		
Water, μg/l (ppm Wt)			5.0E0	5.0E2	1	82	
Land, μg/g (ppm Wt)			1.0E0	1.0E 2	0.2	16	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			58.7		
Water, μg/l (ppm Wt)	1†	100†	290	82	
Land, μg/g (ppm Wt)			0.2	16	

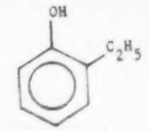
†Phenolic compounds.

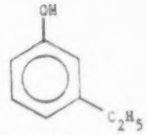
CATEGORY: 18A

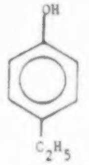
ETHYLPHENOLS: $C_8H_{10}O$ (ethylhydroxy benzenes). 18A080
o-ETHYLPHENOL: (2-ethylphenol). Colorless liquid, with phenolic odor. 18A081
m-ETHYLPHENOL: (3-ethylphenol). A liquid, phenolic odor. 18A082
p-ETHYLPHENOL: (4-ethylphenol). Colorless needles. 18A083

WLN:

STRUCTURE:


o-ethylphenol


m-ethylphenol


p-ethylphenol

PROPERTIES:

	mol.wt.	mp.	bp.	d.	solubility in water
o-ethylphenol	122.17	<-18	207	1.0371^{0}	insoluble
m-ethylphenol	122.17	-4	214	1.0283^{20}_{4}	slightly
p-ethylphenol	122.17	47-8	219	--	slightly

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

TOXIC PROPERTIES, HEALTH EFFECTS:

o-Ethylphenol is reported to have toxic action similar to, but less severe than phenol (ref. 2). Toxicological data for ethylphenols are not available at this time. However, toxicological characteristics are likely to be most similar to those of cresols because of the chemical structure similarity.

Chemical	LD_{50} (oral, rat) (mg/bg)
o-cresol	121
m-cresol	242
p-cresol	207

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 22 mg/m^3 (5 ppm) for cresol (all isomers). NIOSH recommendation is 10 mg/m^3 for cresols.

EPA 1976 Water Quality Criteria: 1 μg/l of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 10).

NAS/NAE 1972 Water Quality Criteria: 1 μg/l of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/l at any time or place; application factor of 0.05 (ref. 4).

U.S. Public Health Service Drinking Water Standards, 1962--Levels for alternate source selection: 1 μg/l (ref. 11).

*** MINIMUM ACUTE TOXICITY CONCENTRATIONS**:

Air, Health: $10 \times 10^3 = 1.0 \times 10^4$ μg/m^3

Water, Health: $5 \times 1 = 5$ μg/l

Land, Health: $0.2 \times 5 = 1$ μg/g

Air, Ecology:

Water, Ecology: $100 \times 5 = 500$ μg/l

Land, Ecology: $0.2 \times 500 = 100$ μg/l

*** ESTIMATED PERMISSIBLE CONCENTRATIONS**:

$EPC_{AH1} = 10^3 \times 10/420 = 24$ μg/m^3

$EPC_{WH1} = 15 \times 24 = 360$ μg/l

$EPC_{WH2} = 13.8 \times 10 = 138$ μg/l

$EPC_{WHS} = 1$ μg/l (phenolic compounds)

$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g

$EPC_{WE1} = 50 \times 1 = 50$ μg/l

$EPC_{WE2} = 1$ μg/l

$EPC_{WES} = 100$ μg/l (phenolic compounds)

$EPC_{LE} = 0.2 \times 1 = 0.2$ μg/g

*Values for health and ecology for ethylphenols are based on data for cresols.

MULTIMEDIA ENVIRONMENTAL GOALS

X
18A080
ETHYLPHENOLS

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent [‡]		B. Ambient Level Goal* [‡]		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.0E4		24		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1.0	1.0	
Land, $\mu g/g$ (ppm Wt)			1.0E0	1.0E2	0.2	0.2	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			24		
Water, $\mu g/l$ (ppm Wt)	1[†]	100[†]	138	1.0	
Land, $\mu g/g$ (ppm Wt)			0.2	0.2	

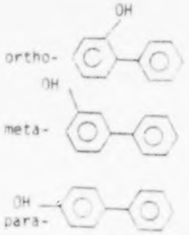
[†] Phenolic compounds.
[‡] Based on data for cresols.

CATEGORY: 18A

WLN: QR BR; QR CR; QR DR

PHENYLPHENOLS: $C_6H_5C_6H_4OH$ (hydroxybiphenyls, biphenylols) 18A100

STRUCTURE:



o-PHENYLPHENOL:	white, flaky crystals; mild, characteristic odor. 18A101
p-PHENYLPHENOL:	needles. 18A102
m-PHENYLPHENOL:	needles. 18A103

PROPERTIES:

Molecular wt: 170.21; insoluble in water.

	mp	bp	d	vap. press.
o-phenylphenol	58-60	286	1.213	1 mm at 100°C
p-phenylphenol	165-167	305-8 sublimes		10 mm at 176°C
m-phenylphenol	78	>300		

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Phenylphenols are monosubstituted phenolic compounds. Ortho, meta, and para phenylphenols are formed.

TOXIC PROPERTIES, HEALTH EFFECTS:

The toxic properties of phenylphenols are probably similar to those of the other phenols. Animal studies indicate that acute and chronic toxicity is mild for o-phenylphenol (ref. 3).

LD_{50} (oral, rat): 2,700 mg/kg (for o-phenylphenol).

Neoplastic effects have resulted from the subcutaneous administration to mice of 1,000 mg/kg of the para isomer. The EPA/NIOSH ordering number is 3101; the adjusted ordering number is 3.1.

Tainting of fish flesh may result from concentrations of 1 mg/ℓ of o-phenylphenol (ref. 4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 10).

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (ref. 4).

U.S. Public Health Service Drinking Water Standards, 1962--Levels for alternate source selection: 1 μg/ℓ (ref. 11).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/3.1 = 2.25 \times 10^4$ μg/m³
Water, Health: $5 \times 1 = 5$ μg/ℓ
Land, Health: $0.2 \times 5 = 1$ μg/g

Air, Ecology:
Water, Ecology: $100 \times 5 = 500$ μg/ℓ
Land, Ecology: $0.2 \times 500 = 100$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 2,700 = 290$ μg/m³
$EPC_{AH3} = 0.081 \times 2,700 = 220$ μg/m³
$EPC_{WH1} = 15 \times 220 = 3,300$ μg/ℓ
$EPC_{WH2} = 0.4 \times 2,700 = 1,080$ μg/ℓ
$EPC_{WHS} = 1$ μg/ℓ (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g
$EPC_{AC1} = 10^3/(6 \times 3.1) = 54$ μg/m³
$EPC_{WC} = 15 \times 54 = 810$ μg/ℓ
$EPC_{LC} = 0.2 \times 810 = 162$ μg/g

$EPC_{WE2} = 1,000$ μg/ℓ (to prevent tainting)
$EPC_{WES} = 100$ μg/ℓ (phenolic compounds)
$EPC_{LE} = 0.2 \times 100 = 20$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

18A100 PHENYLPHENOLS

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.25E4		54		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1.0	100	
Land, $\mu g/g$ (ppm Wt)			1.0E0	1.0E2	0.2	20	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			220		54
Water, $\mu g/l$ (ppm Wt)	1†	100†	1,080	1,000	810
Land, $\mu g/g$ (ppm Wt)			0.2	20	162

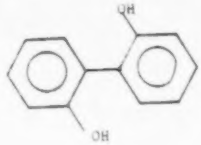
†Phenolic compounds.

CATEGORY: 18A

WLN: QR BR BQ

2,2'-DIHYDROXYDIPHENYL: $C_{12}H_{10}O_2$. (2,2'-biphenyldiol). 18A120

STRUCTURE:



PROPERTIES:

Molecular wt: 186; MP: 109; bp:325-326 ^{755}

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

TOXIC PROPERTIES, HEALTH EFFECTS:

The toxic properties of 2,2'-dihydroxydiphenyl are probably similar to those of other phenols.

LD_{50} (oral, rat): 785 mg/kg for biphenyldiol (ref. 6).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/l of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 10).

NAS/NAE 1972 Water Quality Criteria: 1 μg/l of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent fish tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/l at any time or place; application factor of 0.05 (ref 4).

U.S. Public Health Service Drinking Water Standards, 1962--Levels for alternate source selection: 1 μg/l (ref. 11).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 785 = 3.5 \times 10^4\ \mu g/m^3$

Water, Health: $5 \times 1 = 5\ \mu g/\ell$

Land, Health: $0.2 \times 5 = 1.0\ \mu g/g$

Air, Ecology:

Water, Ecology: $100 \times 5 = 500\ \mu g/\ell$

Land, Ecology: $0.2 \times 500 = 100\ \mu g/g$

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 785 = 84\ \mu g/m^3$

$EPC_{AH3} = 0.081 \times 785 = 63.6\ \mu g/m^3$

$EPC_{WH1} = 15 \times 63.6 = 954\ \mu g/\ell$

$EPC_{WH2} = 0.4 \times 785 = 314\ \mu g/\ell$

$EPC_{WHS} = 1\ \mu g/\ell$ (phenolic compounds)

$EPC_{LH} = 0.2 \times 1 = 0.2\ \mu g/g$

$EPC_{WES} = 100$ (phenolic compounds)

$EPC_{LE} = 0.2 \times 100 = 20\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

18A120
2,2′-DIHYDROXYDIPHENYL

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)			3.5E4		64		
Water, μg/l (ppm Wt)			5.0E0	5.0E2	1	100	
Land, μg/g (ppm Wt)			1.0E0	1.0E2	0.2	20	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

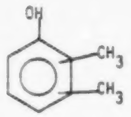
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)			64		
Water, μg/l (ppm Wt)	1†	100†	314		
Land, μg/g (ppm Wt)			0.2	20	

†Phenolic compounds.

CATEGORY: 18A

WLN:

STRUCTURE:



XYLENOLS: $C_8H_{10}O$. (dimethylphenols, dimethylhydroxybenzenes). 18A140

Colorless or white crystals or needles.

2,3-XYLENOL: (1,2-dimethyl-3-hydroxy benzene; 2,3-dimethylphenol). 18A141
2,4-XYLENOL: (2,4-dimethyl-1-hydroxy benzene; 2,4-dimethylphenol). 18A142
2,5-XYLENOL: (1,4-dimethyl-2-hydroxy benzene; 2,5-dimethylphenol). 18A143
2,6-XYLENOL: (1,3-dimethyl-2-hydroxy benzene; 2,6-dimethylphenol). 18A144
3,5-XYLENOL: (1,3-dimethyl-5-hydroxy benzene; 3,5-dimethylphenol). 18A145
3,4-XYLENOL; (1,2-dimethyl-4-hydroxy benzene; 3,4-dimethylphenol). 18A146

PROPERTIES:

	mol wt.	mp	bp	d	vap. press:	water solubility
2,3-XYLENOL	122.17	75	218^{760}	0.9650_4^{20}		slightly
2,4-XYLENOL	122.17	27-8	210^{760}			slightly
2,5-XYLENOL	122.17	75	211.5^{762}			soluble
2,6-XYLENOL	122.17	49	212^{760}			soluble
3,5-XYLENOL	122.17	68	219.5sub	0.9680^{20}	Immat. 62.0°C	soluble
3,4-XYLENOL	122.17	66-8	225^{760}	0.9830_4^{20}		slightly

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Xylenols are disubstituted phenols.

Several isomers are formed since numerous substitution site combinations are possible.

The properties of the various isomers differ somewhat. Xylenols will probably occur in combination.

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxic properties of the xylenols are similar to those of phenol and other phenolic compounds. The lowest LD_{50} (oral, rat) reported for a specific xylenol is 296 mg/kg for 2,6-xylenol. It is probable that mixtures of the various isomers would prove less toxic than 2,6-xylenol.

Oncogenic effects have been reported as a result of animal exposure via skin to five specific xylenol isomers. Considering the compounds collectively the EPA/NIOSH ordering number is 3115, and the lowest dosage resulting in an oncogenic response is 4,000 mg/kg. The adjusted ordering number is 0.8.

Aquatic toxicity: 96-hr LC_{50} for fat head minnow: 14 mg/ℓ (ref. 16).

Tainting of fish flesh may result from concentrations of 1 to 5 mg/ℓ in water (ref. 19).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 10).

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (ref. 4).

U.S. Public Health Service Drinking Water Standards, 1962--Levels for alternate source selection: 1 μg/ℓ (ref. 11).

2,4-Xylenol appears on the EPA Consent Decree List, Priority 2.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 45 x 296 = 1.3×10^4 μg/m^3
Water, Health: 5 x 1 = 5 μg/ℓ
Land, Health: 0.2 x 5 = 1.0 μg/g

Air, Ecology:
Water, Ecology: 100 x 5 = 500 μg/ℓ
Land, Ecology: 0.2 x 500 = 100 μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

EPC_{AH2} = 0.107 x 296 = 32 μg/m^3
EPC_{AH3} = 0.081 x 296 = 24 μg/m^3
EPC_{WH1} = 15 x 24 = 360 μg/ℓ
EPC_{WH2} = 0.4 x 296 = 120 μg/ℓ
EPC_{WHS} = 1 μg/ℓ (phenolic compounds)
EPC_{LH} = 0.2 x 1 = 0.2 μg/g

EPC_{WE1} = 50 x 14,000 = 7×10^5 μg/ℓ
EPC_{WE2} = 1,000 μg/ℓ (to prevent tainting)
EPC_{WES} = 100 μg/ℓ (phenolic compounds)
EPC_{LE} = 0.2 x 100 = 20 μg/g

X
18A140
XYLENOLS

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			1.3E4		24		
Water, μg/l (ppm Wt)			5.0E0	5.0E2	1	100	
Land, μg/g (ppm Wt)			1.0E 0	1.0E2	0.2	20	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			24		
Water, μg/l (ppm Wt)	1[†]	100[†]	120	1,000	
Land, μg/g (ppm Wt)			0.2	20	

[†] Phenolic compounds.

CATEGORY: 18A

ETHYL CRESOLS: $C_9H_{12}O$ (ethyl methylphenols). 18A160

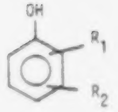
6-ETHYL-m-CRESOL: (6-ethyl-2-methyl phenol). 18A161
4-ETHYL-o-CRESOL: (4-ethyl-3-methyl phenol). 18A162
2-ETHYL-p-CRESOL: (2-ethyl-4-methyl phenol). 18A163

PROPERTIES:

Molecular wt. >136.21; very slightly soluble; higher boiling points than the corresponding xylenols.

WLN:

STRUCTURE: There are 10 possible structural isomers.



R_1 is CH_3

R_2 is C_2H_5

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Ethylcresols are disubstituted phenols, the substitution groups being methyl and ethyl. A number of isomers are possible depending on the substitution sites.

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxic properties are expected to be similar to xylenols.

LD_{50} (rat): 530 mg/kg for 6 ethyl-m-cresol (ref. 6). The route of administration was not reported.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 10).

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (for phenols) (ref. 4).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/ℓ (for phenols) (ref. 11).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 530 = 2.4 \times 10^4$ μg/m^3
Water, Health: $5 \times 1 = 5$ μg/ℓ
Land, Health: $0.2 \times 5 = 1$ μg/g

Air, Ecology:
Water, Ecology: $5 \times 100 = 500$ μg/ℓ
Land, Ecology: $0.2 \times 500 = 100$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 530 = 57$ μg/m^3
$EPC_{AH3} = 0.081 \times 530 = 43$ μg/m^3
$EPC_{WH1} = 15 \times 43 = 640$ μg/ℓ
$EPC_{WH2} = 0.4 \times 530 = 212$ μg/ℓ
$EPC_{WHS} = 1$ μg/ℓ (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g

$EPC_{WES} = 100$ μg/ℓ (phenolic compounds)
$EPC_{LE} = 0.2 \times 100 = 20$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

18A160
ETHYL CRESOLS

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			2.4E4		43		
Water, μg/l (ppm Wt)			5.0E0	5.0E2	1	100	
Land, μg/g (ppm Wt)			1.0E0	1.0E2	0.2	20	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			43		
Water, μg/l (ppm Wt)	1†	100†	212		
Land, μg/g (ppm Wt)			0.2	20	

†Phenolic compounds.

CATEGORY: 18A

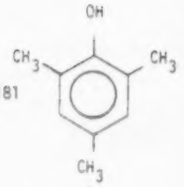
WLN:

POLYALKYL PHENOLS (MW >135): 18A180

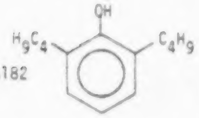
2,4,6-TRIMETHYL PHENOL: $C_9H_{12}O$ (mesitol). 18A181
2,6-DI-sec-BUTYL PHENOL: $C_{14}H_{22}O$. Amber liquid. 18A182
2,6-DIMETHYL-4-HEPTYL PHENOL: $C_{15}H_{24}O$. 18A183

STRUCTURE:

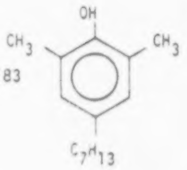
18A181



18A182



18A183



PROPERTIES:

	Mol. wt.	m.p.	b.p.	d
2,4,6-Trimethyl phenol	136.20	72	221	
2,6-Di-sec-butyl phenol	206.3		152-165 at 25 mm	0.936_4^{25}
2,6-Dimethyl-4-heptyl phenol	220.4			

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

2,4,6-Trimethyl phenol has been identified in water samples from two rivers (ref. 21).

TOXIC PROPERTIES, HEALTH EFFECTS:

Details of toxic effects of polyalkyl phenols are not available. They are probably similar to other phenolic compounds.

Compound	LD_{50} (oral, rat)(mg/kg)(ref. 6)
2,4,6-Trimethyl phenol	
2,6-Di-sec-butyl phenol	1,320
2,6-Dimethyl-4-heptyl phenol	1,600

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 10).

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (for phenols) (ref. 4).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/ℓ (for phenols) (ref. 11).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 1{,}320 = 5.9 \times 10^4$ μg/m^3
Water, Health: $5 \times 1 = 5$ μg/ℓ
Land, Health: $0.2 \times 5 = 1$ μg/g

Air, Ecology:
Water, Ecology: $5 \times 100 = 500$ μg/ℓ
Land, Ecology: $0.2 \times 500 = 100$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 1{,}320 = 141$ μg/m^3
$EPC_{AH3} = 0.081 \times 1{,}320 = 107$ μg/m^3
$EPC_{WH1} = 15 \times 107 = 1{,}604$ μg/ℓ
$EPC_{WH2} = 0.5 \times 1{,}320 = 528$ μg/ℓ
$EPC_{WHS} = 1$ μg/ℓ (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g

$EPC_{WES} = 100$ μg/ℓ (phenolic compounds)
$EPC_{LE} = 0.2 \times 100 = 20$ μg/g

18A180
POLYALKYL PHENOLS (MW > 135)

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)			5.9E4		107		
Water, μg/l (ppm Wt)			5.0E0	5.0E2	1	100	
Land, μg/g (ppm Wt)			1.0E0	1.0E2	0.2	20	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)			107		
Water, μg/l (ppm Wt)	1†	100†	528		
Land, μg/g (ppm Wt)			0.2	20	

†Phenolic compounds.

REFERENCES: CATEGORY 18A

Phenols - Monohydrics

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CATEGORY 18

PHENOLS

SUBCATEGORY: 18B - Dihydrics, Polyhydrics

Summary of Subcategory

Total number of compounds in subcategory	4
number of parent compounds with subspecies	0
number of subspecies	0
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

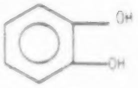
Consent Decree compounds included in subcategory: None

CATEGORY: 18B

WLN: QR BQ

CATECHOL: $C_6H_6O_2$ (pyrocatechol, o-dihydroxybenzene, o-benzenediol, 1,2-dihydroxybenzene, o-hydroxyphenol, 2-hydroxyphenol). White or colorless leaflets. 18B020

STRUCTURE:



PROPERTIES:

Molecular wt: 110.11; mp: 105; bp: 245^{750}; d: 1.344^{21}; soluble; vap. press.: 10 mm at 118.3°; vap. d: 3.79; sublimes readily; soluble in 2.3 parts water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Catechol is a dihydric phenol.

When heated, catechol emits highly toxic fumes; it is volatilized by steam. A related compound is methyl pyrocatechol.

Catechol has been found in onions, in crude beet sugar, in crude wood tar, in drainage water from bituminous shale, in effluents from production of coal-tar chemicals, in coal, and in cigarette smoke (ref. 10).

TOXIC PROPERTIES, HEALTH EFFECTS:

Catechol is similar to phenol in its toxic properties causing convulsions and injury to the blood. It is absorbed through the skin as well as through inhalation (refs. 1, 2).

The repeated absorption of sublethal doses by animals may induce methemoglobinemia, leukopenia, and anemia (ref. 2).

LD_{50} (rats, oral): 3,890 mg/kg.

In skin painting studies in mice, catechol increased the carcinogenic effect of benz(a)pyrene on the skin (ref. 10).

Tainting of fish flesh may result from concentrations of 0.8 to 5 mg/ℓ of catechol (ref. 3).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 20 mg/m^3 (5 ppm) (Trial).

EPA 1976 Water Quality Criteria : 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 4).

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (for phenols) (ref. 3).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/ℓ (for phenols) (ref. 6).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 2.0×10^4 μg/m^3 (5ppm)
Water, Health: 5 x 1 = 5 μg/ℓ
Land, Health: 0.2 x 5 = 1 μg/g

Air, Ecology:
Water, Ecology: 5 x 100 = 500 μg/ℓ
Land, Ecology: 0.2 x 500 = 100 μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 20/420 = 48$ μg/m^3
$EPC_{AH1a} = 5/420 = 0.01$ppm
$EPC_{WH1} = 15 \times 48 = 720$ μg/ℓ
$EPC_{WH2} = 13.8 \times 20 = 280$ μg/ℓ
$EPC_{WHS} = 1$ μg/ℓ (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g

$EPC_{WE2} = 800$ μg/ℓ (to prevent tainting)
$EPC_{WES} = 100$ μg/ℓ (phenolic compounds)
$EPC_{LH} = 0.2 \times 100 = 20$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

18B020
CATECHOL

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.0E4 (5)		48 (0.01)		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1	100	
Land, $\mu g/g$ (ppm Wt)			1.0E 0	1.0E2	0.2	20	

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			48 (0.01)		
Water, $\mu g/l$ (ppm Wt)	1†	100†	280	800	
Land, $\mu g/g$ (ppm Wt)			0.2	20	

†Phenolic compounds.

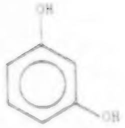
CATEGORY: 18B

1,3-DIHYDROXYBENZENE: $C_6H_4(OH)_2$ (Resorcinol, m-dihydroxybenzene, m-benzenediol). 18B040

A white needle-like crystal with an unpleasant sweet taste.

WLN: QR CQ

STRUCTURE:



PROPERTIES:

Molecular wt: 110.11; mp: 109-111; bp: 280; d: 1.2717^{15}; vap.d: 3.79; vap.press: 1 mm at 108.4°; soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

1,3-Dihydroxybenzene is used in tanning, manufacturing resins, antiseptics, explosives, dyes, and cosmetics, and has been suggested as an aerial bactericide (refs. 6,2).

The threshold limit for the detection of odor in an aqueous solution is 40 mg/l (ref. 2).

The white crystals or tablets turn pink upon exposure to light and air (ref. 2).

1,3-Dihydroxybenzene has been found in wood smoke, in cigarette smoke, in filtered surface and ground water at a water treatment plant, and in the effluents from production of coal-tar chemicals (ref. 10).

TOXIC PROPERTIES, HEALTH EFFECTS:

Skin contact with solutions or salves containing from 3 to 25 percent 1,3-dihydroxybenzene may result in dermatitis and loss of superficial skin layers in humans. Also, methemoglobinemia, convulsions, and death may result. Oral administration produces similar effects. A child complained of dizziness and somnolence after swallowing 4 g. Another child experienced hypothermia, failing blood pressure, and decreased respiration rate after ingesting 8 g (ref. 2). Industrial exposure to 10 ppm produced no discomfort (ref. 4).

1,3-Dihydroxybenzene is readily absorbed from the gastroenteric tract, and, in a suitable solvent, is readily absorbed through the human skin. The substance is excreted in the urine in a free state and conjugated with hexuronic, sulfuric, and other acids (ref. 2).

When tested by repeated skin application, 1,3-dihydroxybenzene showed no carcinogenic effect in mice (ref. 10).

LD_{50} (oral, rat): 301 mg/kg (ref. 6).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 45 mg/m³ (10 ppm)

EPA 1976 Water Quality Criteria: 1 µg/l of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 4).

NAS/NAE 1972 Water Quality Criteria: 1 µg/l of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 µg/l at any time or place, application factor of 0.05 (ref. 3).

U.S. Public Health Service Drinking Water Standards, 1962--Levels for alternate source selection: 1 µg/l (ref. 1).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $10^3 \times 45 = 4.5 \times 10^4$ µg/m³ (10 ppm)

Water, Health: $5 \times 1 = 5$ µg/l

Land, Health: $0.2 \times 5 = 1.0$ µg/g

Air, Ecology:

Water, Ecology: $100 \times 5 = 500$ µg/l

Land, Ecology: $0.2 \times 500 = 100$ µg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 45/420 = 107$ µg/m³

$EPC_{AH1a} = 10/420 = 0.02$ ppm

$EPC_{WH1} = 15 \times 107 = 1{,}605$ µg/l

$EPC_{WH2} = 13.8 \times 45 = 621$ µg/l

$EPC_{WHS} = 1$ µg/l

$EPC_{LH} = 0.2 \times 1 = 0.2$ µg/g

$EPC_{WES} = 100$ µg/l (phenolic compounds)

$EPC_{LE} = 0.2 \times 100 = 20$ µg/g

18B040
1,3-DIHYDROXYBENZENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			4.5E4 (10)		107 (0.02)		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1.0	100	
Land, $\mu g/g$ (ppm Wt)			1.0E0	1.0E2	0.2	20	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			107 (0.02)		
Water, $\mu g/l$ (ppm Wt)	1†	100†	621		
Land, $\mu g/g$ (ppm Wt)			0.2	20	

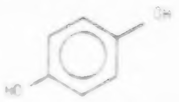
† Phenolic compounds.

WLN: QR DQ

CATEGORY: 188

1,4-DIHYDROXYBENZENE: $C_6H_4(OH)_2$ (hydroquinone, Quinol, p-dihydroxybenzene, 1,4-benzenediol, hydroquinol): 188060
Colorless, hexagonal prisms.

STRUCTURE:



PROPERTIES:

Molecular wt: 110.11; mp: 173-4; bp: 285^{730}; d: 1.328^{15}; vap.d: 3.81; vap press: 1 mm at 132.4°; soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

1,4-Dihydroxybenzene can be formed by the reduction of quinone with sulfurous acid. Uses include photographic developing, and antioxidant. Derivatives of 1,4-dihydroxybenzene include bacteriostatic and tumor-inhibiting agents (ref. 2).

1,4-Dihydroxybenzene in air is usually analyzed by collection in isopropyl alcohol followed by spectrophotometric determination (ref. 2).

Sources of 1,4-dihydroxybenzene include leaves of blueberry, red whortleberry, cranberry, and bearberry (ref. 2).

1,4-Dihydroxybenzene has been found in cigarette smoke and in the effluents from production of coal-tar chemicals (ref. 10).

TOXIC PROPERTIES, HEALTH EFFECTS:

1,4-Dihydroxybenzene produces signs of illness resembling that induced by the other dihydroxybenzenes. In a human adult, ingestion of 1 g may produce nausea, increased respiration rate, and collapse. Skin contact may produce dermatitis. Eye injury has been reported among men exposed to concentrations ranging from 10 to 30 mg/m³. Death, after ingestion of 5 to 12 g, is initiated by respiratory failure (2,7, 8).

Ingestion of "health teas" prepared from the leaves of blueberry, red whortleberry, cranberry, or bearberry should be avoided because the leaf may contain large amounts of 1,4-dihydroxybenzene capable of producing systemic poisoning (ref. 2).

1,4-dihydroxybenzene is absorbed more readily than phenol from the gastroenteric tract. The compound is oxidized in the body to the more toxic quinone (ref. 2).

LD_{50} (oral, rat): 320 mg/kg (ref. 8).

1,4-Dihydroxybenzene was found inactive as an initiator of skin carcinogenesis (ref. 10).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 2 mg/m³ (0.44 ppm).

Hydruqqinone is the subject of a NIOSH Criteria document. The NIOSH recommendation for occupational exposure is 2 mg/m³ as a 15 minute ceiling (ref. 11).

EPA 1976 Water Quality Criteria: 1 µg/l of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 4).

NAS/NAE 1972 Water Quality Criteria: 1 µg/l of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 µg/l at any time or place; application factor of 0.05 (ref. 3).

U.S. Public Health Service Drinking Water Standards, 1962--Levels for alternate source selection: 1 µg/l (for phenols)(ref. 1).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $10^3 \times 2 = 2{,}000\ \mu g/m^3$ (0.44 ppm)
Water, Health: $5 \times 1 = 5\ \mu g/l$
Land, Health: $0.2 \times 5 = 1.0\ \mu g/g$

Air, Ecology:
Water, Ecology: $100 \times 5 = 500\ \mu g/l$
Land, Ecology: $0.2 \times 500 = 100\ \mu g/g$

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 2/420 = 4.76\ \mu g/m^3$
$EPC_{AH1a} = 0.44/420 = 1.0 \times 10^{-3}$ ppm
$EPC_{WH1} = 15 \times 4.76 = 71.4\ \mu g/l$
$EPC_{WH2} = 13.8 \times 2 = 27.6\ \mu g/l$
$EPC_{WHS} = 1\ \mu g/l$ (phenolic compound)
$EPC_{LH} = 0.2 \times 1.0 = 0.2\ \mu g/g$

$EPC_{WES} = 100\ \mu g/l$ (phenolic compounds)
$EPC_{LE} = 0.2 \times 100 = 20\ \mu g/g$

188

MULTIMEDIA ENVIRONMENTAL GOALS

X
18B060
1,4-DIHYDROXYBENZENE

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.0E3 (0.44)		4.8 (0.001)		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1	100	
Land, $\mu g/g$ (ppm Wt)			1.0E0	1.0E2	0.2	20	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

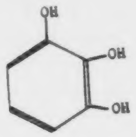
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			4.8 (0.001)		
Water, $\mu g/l$ (ppm Wt)	1†	100†	27.6		
Land, $\mu g/g$ (ppm Wt)			0.2	20	

†Phenolic Compounds

WLN: QR BQ CQ

CATEGORY: 18B
1,2,3-TRIHYDROXYBENZENE: $C_6H_6O_3$ 18B080
(1,2,3-benzenetriol, pyrogallic acid, pyrogallol).
White, odorless crystal.

STRUCTURE:



PROPERTIES:

Molecular wt: 126.11; mp: 133-4; bp: 309^{760}; d: 1.453_4^4;
Vap. press: 10 mm at 167.7^0; soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

1,2,3-trihydroxybenzene is used as a developer in photography, as mordant for wool, staining leather, manufacturing dyes, and in adsorption of oxygen in gas analysis, and for maintaining anaerobic conditions for bacterial growth. It is a product of *Penicillium patulum* (ref. 8).

TOXIC PROPERTIES, HEALTH EFFECTS:

Ingestion of 1,2,3-trihydroxybenzene may produce severe G.I. irritation, renal and hepatic damage, and death (ref. 6). Death is initiated by respiratory failure because it ties up oxygen in the blood (ref. 2).

Cases of human poisoning include one man who ingested 8 g and recovered, and one man who ingested 15 g and subsequently died. Skin contact may result in sensitization and death (ref. 2).

LD_{50} (oral, rat): 789 mg/kg (ref. 8).

Concentrations of 20 to 30 mg/l in water result in tainting of fish flesh (ref. 3). 1,2,3-trihydroxybenzene has been reported to demonstrate cocarcinogenic activity (ref. 9).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/l of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 4).

NAS/NAE 1972 Water Quality Criteria: 1 μg/l of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/l at any time or place; application factor of 0.05 (ref. 3).

U.S. Public Health Service Drinking Water Standards, 1962--Levels for alternate source selection: 1 μg/l (ref. 5).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 789 = 3.55 \times 10^4$ μg/m^3
Water, Health: $5 \times 1 = 5$ μg/l
Land, Health: $0.2 \times 5 = 1.0$ μg/g

Air, Ecology:
Water, Ecology: $100 \times 5 = 500$ μg/l
Land, Ecology: $0.2 \times 500 = 100$μμg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 789 = 84.4$ μg/m^3
$EPC_{AH3} = 0.081 \times 789 = 63.9$ μg/m^3
$EPC_{WH1} = 15 \times 63.9 = 959$ μg/l
$EPC_{WH2} = 0.4 \times 789 = 316$ μg/l
$EPC_{WES} = 1$ μg/l (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g

$EPC_{WE2} = 2.0 \times 10^4$ μg/l
$EPC_{WES} = 100$ μg/l (phenolic compounds)
$EPC_{LE} = 0.2 \times 100 = 20$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

18B080

1,2,3-TRIHYDROXYBENZENE

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			3.55E4		63.9		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1	100	
Land, $\mu g/g$ (ppm Wt)			1.0E0	1.00E2	0.2	20	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			63.9		
Water, $\mu g/l$ (ppm Wt)	1†	100 †	316	20,000	
Land, $\mu g/g$ (ppm Wt)			0.2	20	

†Phenolic compounds.

REFERENCES: CATEGORY 18B

Phenols - Dihydrics, Polyhydrics

1. Sax, N. I., Ed. Dangerous Properties of Industrial Materials, Fourth Edition. Van Nostrand Reinhold Co., New York, NY (1975).

2. Deichmann, W. B., and M. L. Keplinger. Phenols and Phenolic Compounds. Industrial Hygiene and Toxicology, Second Revised Edition, Vol. 2, F. A. Patty, Ed., Interscience Publishers, New York, NY (1963).

3. National Academy of Sciences, National Academy of Engineering. Water Quality Criteria 1972. A Report. National Academy of Sciences, Washington, DC. EPA-R3-73-033 (1973).

4. U.S. Environmental Protection Agency. Quality Criteria for Water. EPA 440/9-76-023 (1976).

5. U.S. Public Health Service. Drinking Water Standards: 1962. Title 42 Code Federal Regulations, Part 72.

6. Windholz, M., Ed. The Merck Index: An Encyclopedia of Chemicals and Drugs, Ninth Edition. Merck & Co., Inc., Rahway, NJ (1976).

7. American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values for Substances in Workroom Air with Supplements, Third Edition. American Conference of Governmental Industrial Hygienists, Cincinnati, OH (1974).

8 Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

9. Lawley, P. D. Carcinogenesis by Alkylating Agents. Chemical Carcinogens. ACS Monograph 173, C. E. Searle, Ed., Am. Chem. Soc., Washington, DC (1976).

10. International Agency for Research on Cancer. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Man, Vol. 15, Lyon, France. A World Health Organization Publication (WHO), Geneva (1977).

11. National Institute for Occupational Safety and Health. Criteria for a Recommended Standard Occupational Exposure to Hydroquinone (1978). Available from Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. GPO 757-141-6799. DHEW (NIOSH) Publication No. 78-155.

CATEGORY 18

PHENOLS

SUBCATEGORY: 18C - Fused Ring Hydroxy Compounds

Summary of Subcategory

Total number of compounds in subcategory	13
number of parent compounds with subspecies	2
number of subspecies	8
Number of parent compounds with no MEG values	3
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

Consent Decree compounds included in subcategory: None

193<

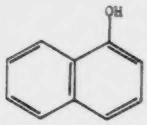
CATEGORY: 18C

1-NAPHTHOL: $C_{10}H_8O$ (α-naphthol, α-hydroxynaphthalene, 1-naphthalenol). 18C020

A colorless or yellow powder with a phenolic odor and a disagreeable, burning taste.

WLN: L66J BQ

STRUCTURE:



PROPERTIES:

Molecular wt. 144.19; mp: 96; bp: 288^{760}; d: 1.0989^{99}_{4}; vap.press: 1 mm at 94°; slightly soluble in hot water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

1-Naphthol is used in manufacturing dyes, intermediates, synthetic perfumes, and in microscopy. It can be formed by oxidation of naphthalene (ref. 1).

The threshold limit for the detection of odor in aqueous solution is 7.0 mg/l (ref. 2).

TOXIC PROPERTIES, HEALTH EFFECTS:

In humans, 1-naphthol has been shown to produce gastrointestinal tract disturbance, convulsions, and death when ingested. Also, sufficient naphthol may be absorbed through the skin to cause kidney irritation and eye injury (ref. 3).

LD_{50} (oral, rat): 2,590 mg/kg (ref. 4).

Tainting of fish flesh may result from a concentration of 500 μg/l in water (ref. 5).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/l of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 6).

NAS/NAE 1972 Water Quality Criteria: 1 μg/l of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/l at any time or place: application factor of 0.05 (ref. 5).

U.S. Public Health Service Drinking Water Standards, 1962--Levels for alternate source selection: 1 μg/l (ref. 7).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 2{,}590 = 1.17 \times 10^5$ μg/m^3

Water, Health: $5 \times 1 = 5$ μg/l

Land, Health: $0.2 \times 5 = 1$ μg/g

Air, Ecology:

Water, Ecology: $100 \times 5 = 500$ μg/l

Land, Ecology: $0.2 \times 500 = 100$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 2{,}590 = 277$ μg/m^3

$EPC_{AH3} = 0.081 \times 2{,}590 = 210$ μg/m^3

$EPC_{WH1} = 15 \times 210 = 3{,}150$ μg/l

$EPC_{WH2} = 0.4 \times 2{,}590 = 1{,}036$ μg/l

$EPC_{WHS} = 1$ μg/l (phenolic compounds)

$EPC_{LH} = 0.2 \times 1.0 = 0.2$ μg/g

$EPC_{WE2} = 500$ μg/l (to prevent tainting)

$EPC_{WES} = 100$ μg/l (phenolic compounds)

$EPC_{LE} = 0.2 \times 100 = 20$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

18C020
1-NAPHTHOL

EMISSION LEVEL GOALS	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, µg/m^3 (ppm Vol)			1.17E5		210		
Water, µg/l (ppm Wt)			5.0E0	5.0E2	1	100	
Land, µg/g (ppm Wt)			1.0E0	1.0E2	0.2	20	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, µg/m^3 (ppm Vol)			210		
Water, µg/l (ppm Wt)	1 †	100 †	1,036	500	
Land, µg/g (ppm Wt)			0.2	20	

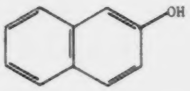
† Phenolic Compounds

CATEGORY: 18C

2-NAPHTHOL: $C_{10}H_8O$ (2-hydroxy naphthalene, β-naphthol, β-naphthyl hydroxide). 18C040
A white to yellowish-white powder or crystals with a phenolic odor.

WLN: L66J CQ

STRUCTURE:



PROPERTIES:
Molecular wt: 144.19; mp: 123-4; bp: 295^{760}; d: 1.28^{20}; vap.d: 4.97; vap.press: 10 mm at 145.5°; insoluble in cold water, slightly soluble in hot water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

2-Naphthol is used in manufacturing medicinal organics, dyes, and perfumes. The largest single use is reported to be in the rubber industry, where it is used in making antioxidants. The substance darkens with age when exposed to light (ref. 1).
2-Naphthol can be formed by oxidation of naphthalene (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

Ingestion of large amounts of 2-naphthol by humans may produce gastrointestinal tract disturbances, kidney damage, circulatory collapse, and death. Also, fatal poisoning resulting from external application has been reported (ref. 1).
LD_{50} (oral, rat): 2,420 mg/kg (ref. 4).
Tainting of fish flesh may result from a concentration of 300 μg/l in water (ref. 5).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/l of phenol (including phenolic compounds for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 6).
NAS/NAE 1972 Water Quality Criteria: 1 μg/l of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/l at any time or place; application factor of 0.05 (ref. 5).
U.S. Public Health Service Drinking Water Standards, 1962--Levels for alternate source selection: 1 μg/l (ref. 7).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 2{,}420 = 1.09 \times 10^5\ \mu g/m^3$
Water, Health: $5 \times 1 = 5\ \mu g/l$
Land, Health: $0.2 \times 5 = 1\ \mu g/g$

Air, Ecology:
Water, Ecology: $100 \times 5 = 500\ \mu g/l$
Land, Ecology: $0.2 \times 500 = 100\ \mu g/l$

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 2{,}420 = 259\ \mu g/m^3$
$EPC_{AH3} = 0.081 \times 2{,}420 = 196\ \mu g/m^3$
$EPC_{WH1} = 15 \times 196 = 2{,}940\ \mu g/l$
$EPC_{WH2} = 0.4 \times 2{,}420 = 968\ \mu g/l$
$EPC_{WHS} = 1\ \mu g/l$ (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = 0.2\ \mu g/g$

$EPC_{WE2} = 300\ \mu g/l$ (to prevent tainting)
$EPC_{WES} = 100\ \mu g/l$ (phenolic compounds)
$EPC_{LE} = 0.2 \times 100 = 20\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

18C040
2-NAPHTHOL

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.09E5		196		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1	100	
Land, $\mu g/g$ (ppm Wt)			1.0E0	1.0E2	0.2	20	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			196		
Water, $\mu g/l$ (ppm Wt)	1†	100†	968	300	
Land, $\mu g/g$ (ppm Wt)			0.2	20	

†Phenolic compounds.

CATEGORY: 18C

PHENANTHROLS: $C_{14}H_{10}O$ (hydroxyphenanthrenes). 18C060

1-HYDROXYPHENANTHRENE: A solid. 18C061
2-HYDROXYPHENANTHRENE: A solid. 18C062
3-HYDROXYPHENANTHRENE: A solid. 18C063
4-HYDROXYPHENANTHRENE: A solid. 18C064
9-HYDROXYPHENANTHRENE: A solid. 18C065

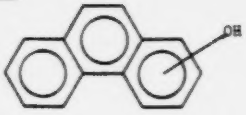
PROPERTIES:	mol wt	mp.	solubility in water
1-hydroxyphenanthrene	194.24	156	
2-hydroxyphenanthrene	194.24	169	
3-hydroxyphenanthrene	194.24	122-3	
4-hydroxyphenanthrene	194.24	113	
9-hydroxyphenanthrene	194.24	152-3	slight

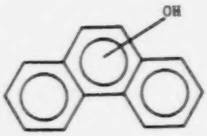
NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Five isomers for phenanthrols are possible.

WLN:

STRUCTURE:





TOXIC PROPERTIES, HEALTH EFFECTS:

The compounds 2-, 3-, and 9-phenanthrol are reported to be an analgesic and exert a depressing action on experimental animals (ref. 8).

Specific toxicity data are not currently available.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

18C060
PHENANTHROLS

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

CATEGORY: 18C

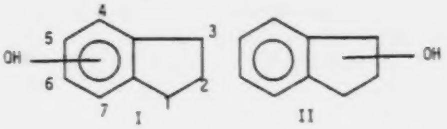
WLN: L56T&J GQ

INDANOLS: $C_9H_{10}O$ (hydroxyhydrindene, hydroxyindan).

Plates, triclinic prisms, or needles. 18C080

1-INDANOL. 18C081
4-INDANOL. 18C082
5-INDANOL. 18C083

STRUCTURE:



PROPERTIES:

	Molecular wt.	mp	bp	Water solubility
1-INDANOL	134.18	54	255	slightly soluble
4-INDANOL	134.18	40,50	120,128	...
5-INDANOL	134.18	56	255	slightly soluble

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPCUNDS:

Indanol may or may not be phenolic, depending on the site of hydroxy substitution. Structure I is a phenol, II is not. Little information regarding indanols is available.

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxic properties are probably similar to but milder than phenol. Limited animal experiments suggest moderate toxicity and a high degree of irritation (ref. 3).

LD_{50} (oral, rat): 3,250 mg/kg for a 5-indanol.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria : 1 µg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 6).

NAS/NAE 1972 Water Quality Criteria: 1 µg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 µg/ℓ at any time or place; application factor of 0.05 (for phenols) (ref. 5).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 µg/ℓ (for phenols) (ref. 7).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 3{,}250 = 1.5 \times 10^5$ µg/m^3
Water, Health: $5 \times 1 = 5$ µg/ℓ
Land, Health: $0.2 \times 5 = 1$ µg/g

Air, Ecology:
Water, Ecology: $5 \times 100 = 500$ µg/ℓ
Land, Ecology: $0.2 \times 500 = 100$ µg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 3{,}250 = 350$ µg/m^3
$EPC_{AH3} = 0.081 \times 3{,}250 = 260$ µg/m^3
$EPC_{WH1} = 15 \times 260 = 3{,}900$ µg/ℓ
$EPC_{WH2} = 0.4 \times 3{,}250 = 1{,}300$ µg/ℓ
$EPC_{WHS} = 1$ µg/ℓ (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = 0.2$ µg/g

$EPC_{WES} = 100$ µg/ℓ (phenolic compounds)
$EPC_{LE} = 0.2 \times 100 = 20$ µg/g

MULTIMEDIA ENVIRONMENTAL GOALS

18C080
INDANOLS

EMISSION LEVEL GOALS	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.5E5		260		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1	100	
Land, $\mu g/g$ (ppm Wt)			1.0E0	1.0E2	0.2	20	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			260		
Water, $\mu g/l$ (ppm Wt)	1†	100†	1,300		
Land, $\mu g/g$ (ppm Wt)			0.2	20	

†Phenolic compounds.

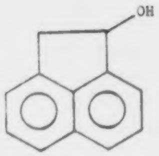
201<

CATEGORY: 18C

1-ACENAPHTHOL: $C_{12}H_{10}O$. 18C100

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt; 170.21; mp: 147-148

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for 1-acenaphthol are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

18C100
1-ACENAPHTHOL

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

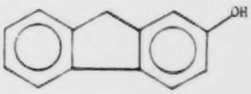
AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

CATEGORY: 18C
2-HYDROXYFLUORENE: $C_{13}H_{10}O$ (2-fluorenol) 18C120
A solid crystal.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 182.23; mp: 171-4; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

2-Hydroxyfluorene occurs in the anthracene oil fraction of coal-tar distillate boiling from 340 to 370° (ref. 9).

The compound may occur as a constituent of particulate polycyclic aromatic hydrocarbons, PPAH.

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for 2-hydroxyfluorene are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

18C120
2-HYDROXYFLUORENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

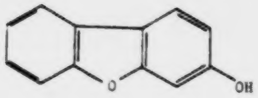
*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

CATEGORY: 18C
2-HYDROXYDIBENZOFURAN: $C_{11}H_7O_2$. 18C140
A solid.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 171.056.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

The compound may occur as a constituent of particulate polycyclic aromatic hydrocarbons, PPAH.

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for 2-hydroxydibenzofuran are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

18C140
2-HYDROXYDIBENZOFURAN

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

REFERENCES: CATEGORY 18C

Phenols - Fused Ring Hydroxy Compounds

1. Windholz, M., Ed. The Merck Index: An Encyclopedia of Chemicals and Drugs, Ninth Edition. Merck & Co., Inc., Rahway, NJ (1976).

2. Deichmann, W. B., and M. L. Keplinger. Phenols and Phenolic Compounds. Industrial Hygiene and Toxicology, Second Revised Edition, Vol. 2, F. A. Patty, Ed., Interscience Publishers, New York, NY (1963).

3. Sax, N. I., Ed. Dangerous Properties of Industrial Materials, Fourth Edition. Van Nostrand Reinhold Co., New York, NY (1975).

4. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

5. National Academy of Sciences, National Academy of Engineering. Water Quality Criteria 1972. A Report. National Academy of Sciences, Washington, DC. EPA-R3-73-033 (1973).

6. U.S. Environmental Protection Agency. Quality Criteria for Water. EPA 400/9-76-023 (1976).

7. U.S. Public Health Service. Drinking Water Standards: 1962. Title 42 Code Federal Regulations, Part 72.

8. Eddy, N. B. Studies of Phenanthrene Derivatives I. A Comparison of Phenanthrene and Some 2, 3, and 9 Monosubstituted Products. Journal Pharmacology 48 (1933).

9. Kruber, R. Chemische Berichte, Vol. 69, P. 107.

CATEGORY 19

HALOGENATED PHENOLIC COMPOUNDS

SUBCATEGORY: 19A - Halophenols

Summary of Subcategory

Total number of compounds in subcategory	4
number of parent compounds with subspecies	0
number of subspecies	0
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	2

Consent Decree compounds included in subcategory: 4

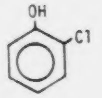
19A020	2-Chlorophenol
19A040	2,4-Dichlorophenol
19A050	2,4,6-Trichlorophenol
19A060	Pentachlorophenol

CATEGORY: 19A

WLN: QR BG

2-CHLOROPHENOL: C_6H_5OCl (o-chlorophenol). 19A020
Light amber liquid; distinct odor.

STRUCTURE:



PROPERTIES:

Molecular wt: 128.6; mp: 9.0; bp: 174.9; d: 1.263; vap. press.: 1 mm at 12.1°C; solubility in water: 2.85 g in 100 ml at 20°.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

The chlorophenols are primarily water and soil contaminants.

Chlorination of phenols in aqueous solution can occur under conditions similar to those used in chlorine disinfection (ref. 1).

Chlorophenols are stronger acids than phenols because of the chlorine atoms. They, like phenols, will form ethers, esters, and salts with metals, amines, etc.

Aqueous photolysis may lead to hydroxyl substitution for the chlorines and polymer formation.

In terms of biological degradation, chlorophenols are much more environmentally stable than the parent phenol. Microbial decomposition of 2-chlorophenol required 3 to 9 days for complete disappearance as compared to 1 to 2 days for phenol (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

Chlorophenols may be absorbed through the skin as well as by inhalation of the vapors. They are considered corrosive to skin and eyes, and the vapors are irritating and toxic.

LD_{50} (oral, rat): 670 mg/kg.

2-chlorophenol is reported to produce tumors when 38 g/kg was applied to the skin of mice. The NIOSH ordering number is 3,121, and the adjusted ordering number is 0.09.

Concentrations of 0.0001 to 0.015 mg/ℓ in water may cause tainting of fish flesh (refs. 3,4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 3)..

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (ref. 4).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/ℓ (for phenols) (ref. 5).

Candidate for the list for Toxic Pollutant Effluent Limitations (ref. 6). On EPA Consent Decree Priority II List.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 670 = 3.0 \times 10^4$ μg/m^3
Water, Health: $5 \times 1 = 5$ μg/ℓ
Land, Health: $0.2 \times 5 = 1$ μg/g

Air, Ecology:
Water, Ecology: $5 \times 100 = 500$ μg/ℓ
Land, Ecology: $0.2 \times 500 = 100$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 670 = 72$ μg/m^3
$EPC_{AH3} = 0.081 \times 670 = 54$ μg/m^3
$EPC_{WH1} = 15 \times 54 = 810$ μg/ℓ
$EPC_{WH2} = 0.4 \times 670 = 270$ μg/ℓ
$EPC_{WHS} = 1$ μg/ℓ (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g

$EPC_{WE2} = 0.1$ μg/ℓ (to prevent tainting)
$EPC_{WES} = 100$ μg/ℓ (phenolic compounds)
$EPC_{LE} = 0.2 \times 0.1 = 0.02$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

19A020
2-CHLOROPHENOL

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			3.0E4		54		
Water, μg/l (ppm Wt)			5.0E0	5.0E2	1	0.1	
Land, μg/g (ppm Wt)			1.0E 0	1.0E2	0.2	0.02	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			54		
Water, μg/l (ppm Wt)	1†	100†	270	0.1	
Land, μg/g (ppm Wt)			0.2	0.02	

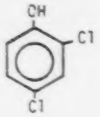
† Phenolic compounds.

CATEGORY: 19A

WLN: QR BG DG

2,4-DICHLOROPHENOL: $C_6H_4OCl_2$. 19A040
Colorless crystals.

STRUCTURE:



PROPERTIES:

Molecular wt: 163.0; mp: 45; bp: 210-211; d: 1.383_{25}^{60}; vap. d.: 5.62; vap. press: 1 mm at 53° C; solubility in water: 0.45 g in 100 ml at 20°.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

The chlorophenols are primarily water and soil contaminants. Chlorination of phenols in an aqueous solution can occur under conditions similar to those used in chlorine disinfection (refs. 1,4). Chlorophenols are stronger acids than phenols because of the chlorine atoms. They, like phenols, will form ethers, esters, and salts with metals, amines, etc. They have been identified in samples of U.S. drinking water supplies at 36 μg/ℓ (ref. 7).

In terms of biological degradation the chlorophenols are much more environmentally stable than the parent phenol. The rate of decomposition further decreases as the number of chlorine atoms increases. Microbial decomposition of 2,4-dichlorophenol required 5 to 9 days for complete disappearance as compared to 1 to 2 days required for phenol (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

Chlorophenols may be absorbed through skin as well as by inhalation of the vapors. They are considered corrosive to skin and eyes, and vapors are irritating and toxic. Dichlorophenols are more toxic than monochlorophenols (ref. 2).

LD_{50}(oral, rat): 580 mg/kg.

2,4-dichlorophenol is reported to cause cancer in mice. The EPA/NIOSH ordering number is 3121. The lowest dose affecting an oncogenic response is 312 mg/kg. The adjusted ordering number is 10.

Concentrations of 0.0004 to 0.014 mg/ℓ in water may cause tainting of fish flesh (refs. 3,4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 3).

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (ref. 4).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/ℓ (for phenols) (ref. 5).

On EPA Consent Decree Priority II List.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/10 = 7 \times 10^3$ μg/m^3
Water, Health: 5 x 1 = 5 μg/ℓ
Land, Health: 0.2 x 5 = 1 μg/g

Air, Ecology:
Water, Ecology: 5 x 100 = 500 μg/ℓ
Land, Ecology: 0.2 x 500 = 100 μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

EPC_{AH2} = 0.107 x 580 = 62 μg/m^3
EPC_{AH3} = 0.081 x 580 = 47 μg/m^3
EPC_{WH1} = 15 x 47 = 705 μg/ℓ
EPC_{WH2} = 0.4 x 580 = 232 μg/ℓ
EPC_{WHS} = 1 μg/ℓ (phenolic compounds)
EPC_{LH} = 0.2 x 1 = 0.2 μg/g
EPC_{AC2} = $10^3/(6 \times 10)$ = 17 μg/m^3
EPC_{WC} = 15 x 17 = 255 μg/ℓ
EPC_{LC} = 0.2 x 255 = 51 μg/g

EPC_{WE2} = 0.4 μg/ℓ (to prevent tainting)
EPC_{WES} = 100 μg/ℓ (phenolic compounds)
EPC_{LE} = 0.2 x 0.4 = 0.08 μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

19A040
2,4-DICHLOROPHENOL

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			7.0E3		17		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1	0.4	36‡
Land, $\mu g/g$ (ppm Wt)			1.0E0	1.0E2	0.2	0.08	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			47		17
Water, $\mu g/l$ (ppm Wt)	1†	100†	232	0.4	255
Land, $\mu g/g$ (ppm Wt)			0.2	0.08	51

†Phenolic compounds.

‡Highest level identified in drinking water supplies.

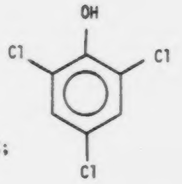
CATEGORY: 19A

WLN: QR BG DG FG

2,4,6-TRICHLOROPHENOL: $C_6H_3Cl_3O$. 19A050

Colorless needles or yellow solid; a strong phenolic odor.

STRUCTURE:



PROPERTIES:

Molecular wt: 197.46; mp: 68; bp: 246; d: 1.490 (75°/4°); vap. press: 1 mm at 76.5°C; solubility in water: 800 mg/ℓ at 25°C.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

2,4,6-Trichlorophenol is manufactured for use as a fungicide, bactericide, and wood preservative (ref. 2). It is prepared by the direct chlorination of phenol (ref. 9).

TOXIC PROPERTIES, HEALTH EFFECTS:

Oral administration in rats causes restlessness, increased rate of respiration, motor weakness, tremors, clonic convulsions dyspnea, coma, and death.

LD_{50} (oral, rat): 820 mg/kg.

2,4,6-Trichlorophenol is reported to cause cancer in mice. The EPA/NIOSH ordering number is 3111. The lowest dosage to induce tumors is 29 grams/kg (ref. 11). The adusted ordering number is 0.107.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 3).

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time of place; application factor of 0.05 (ref. 4).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/ℓ (for phenols) (ref. 5).

2,4,6-Trichlorophenol appears on EPA Consent Decree List, Priority 3.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 820 = 3.7 \times 10^4\ \mu g/m^3$

Water, Health: $5 \times 1 = 5\ \mu g/\ell$

Land, Health: $0.2 \times 5 = 1\ \mu g/g$

Air, Ecology:

Water, Ecology: $5 \times 100 = 500\ \mu g/\ell$

Land, Ecology: $0.2 \times 500 = 100\ \mu g/g$

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 820 = 88\ \mu g/m^3$

$EPC_{AH3} = 0.081 \times 820 = 66\ \mu g/m^3$

$EPC_{WH1} = 15 \times 66 = 996\ \mu g/\ell$

$EPC_{WH2} = 0.4 \times 820 = 328\ \mu g/\ell$

$EPC_{WHS} = 1\ \mu g/\ell$ (phenolic compounds)

$EPC_{LH} = 0.2 \times 1 = 0.2\ \mu g/g$

$EPC_{WE2} = 0.1\ \mu g/\ell$ (to prevent tainting)

$EPC_{WES} = 100\ \mu g/\ell$ (phenolic compounds)

$EPC_{LE} = 0.2 \times 0.1 = 0.02\ \mu g/g$

214<

MULTIMEDIA ENVIRONMENTAL GOALS

19A050
2,4,6-TRICHLOROPHENOL

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			3.7E4		66		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1	0.1	
Land, $\mu g/g$ (ppm Wt)			1.0E0	1.0E2	0.2	0.02	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			66		
Water, $\mu g/l$ (ppm Wt)	1†	100†	328	0.1	
Land, $\mu g/g$ (ppm Wt)			0.2	0.02	

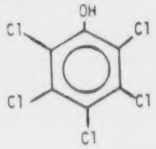
†Phenolic Compounds.

CATEGORY: 19A

PENTACHLOROPHENOL: Cl_5C_6OH(chlorophen). 19A060
White, monoclinic cyrstals that have a pungent odor when hot.

WLN:

STRUCTURE:



PROPERTIES:
Molecular wt: 266.34; mp: 174; bp: $309\text{-}10^{754}$; d: 1.978^{22}_{4}; vap.press: 40 mm at 211.2°; slightly soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Pentachlorophenol has been reported in samples taken from lake water and from public drinking water (ref. 8). The highest concentration reported in drinking water is 1.4 µg/l (ref. 7).

Pentachlorophenol is used as an insecticide for termite control, as a general herbicide, and as a fungicide (refs. 9,10).

Pentachlorophenol in water and tissue can be determined spectrophotometrically. It is prepared by the chlorination of phenol (ref. 2).

TOXIC PROPERTIES, HEALTH EFFECTS:

Pentachlorophenol in dust (0.3 mg/m^3) is irritating to mucous membranes (ref. 12). Ingestion causes respiratory irregularity and may cause convulsions and death (29 mg/kg has caused human death)(ref. 11). Ingestion causes lung, liver, and kidney damage (ref. 9). Skin irritation is reported as a result of brief single exposures to solutions containing more than 10 percent of the compound (ref. 2).

Pentachlorophenol can be absorbed from the gastrointestinal tract and through the skin. The compound is believed to cause a radical uncoupling of oxidation and phosphorylation cycles in tissues, which produces an increased metabolic rate and increased temperature (ref. 2).

LD_{50} (oral, rat): 50 mg/kg (ref. 11).

Pentachlorophenol has been found to cause tumors in mice. The EPA/NIOSH ordering number is 3,101. The lowest effective dosage is 46 mg/kg, and the adjusted ordering number is 67.

Aquatic toxicity: Median threshold limit for clam eggs and larvae is <250 ppb (ref. 4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.5 mg/m^3 (0.046 ppm).

EPA 1976 Water Quality Criteria: 1 µg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 3).

NAS/NAE 1972 Water Quality Criteria: 1 µg/l of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 µg/l at any time or place; application factor of 0.05 (ref. 4).

U.S. Public Health Service Drinking Water Standards, 1962--Levels for alternate source selection: 1 µg/l (for phenols) (ref. 5).

Pentachlorophenol is included in the EPA Consent Decree List, Priority II.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $10^3 \times 0.5 = 500\ \mu g/m^3$ (0.046 ppm)

Water, Health: $5 \times 1 = 5\ \mu g/l$

Land, Health: $0.2 \times 5 = 1.0\ \mu g/g$

Air, Ecology:

Water, Ecology: $100 \times 0.25 = 25\ \mu g/l$

Land, Ecology: $0.2 \times 25 = 5\ \mu g/g$

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 0.5/420 = 1.2\ \mu g/m^3$
$EPC_{AH1a} = 0.046/420 = 1.1 \times 10^{-4}$ ppm
$EPC_{WH1} = 15 \times 1.2 = 18\ \mu g/l$
$EPC_{WH2} = 13.8 \times 0.5 = 6.9\ \mu g/l$
$EPC_{WHS} = 0.2 \times 1 = 1\ \mu g/l$ (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = 0.2\ \mu g/g$
$EPC_{AC2} = 10^3/(6 \times 67) = 2.5\ \mu g/m^3$
$EPC_{WC} = 15 \times 2.5 = 37\ \mu g/l$
$EPC_{LC} = 0.2 \times 37 = 7.4\ \mu g/g$

$EPC_{WE1} = 50 \times 0.25 = 12.5\ \mu g/l$
$EPC_{WES} = 100\ \mu g/l$(phenolic compounds)
$EPC_{LE} = 0.2 \times 12.5 = 2.5\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

X
19A060
PENTACHLOROPHENOL

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			5.0E2		1.2 (1.1×10^{-4})		
Water, μg/l (ppm Wt)			5.0E0	2.5 E1	1	12.5	1.4†
Land, μg/g (ppm Wt)			1.0E0	5.0E0	0.2	2.5	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			1.2 (1.1×10^{-4})		2.5
Water, μg/l (ppm Wt)	1‡	100 ‡	6.9	12.5	37
Land, μg/g (ppm Wt)			0.2	2.5	7.4

† Highest concentration identified in drinking water.

‡ Phenolic compounds.

REFERENCES: CATEGORY 19A

Halogenated Phenolic Compounds - Halophenols

1. Howard, P. H., and P. R. Durkin. Preliminary Hazard Assessment of Chlorinated Naphthalenes, Silicones, Fluorocarbons, Benzenepolycarboxylates, and Chlorophenols. Prepared by Syracuse University Research Corporation under Contract No. 68-01-2202 for Environmental Protection Agency. Available from National Technical Information Service, U.S. Department of Commerce, Springfield, VA. PB 238 074 (1973).

2. Deichmann, W. B., and M. L. Keplinger. Phenols and Phenolic Compounds. *Industrial Hygiene and Toxicology, Second Revised Edition, Vol. 2*, F. A. Patty, Ed., Interscience Publishers, New York, NY (1963).

3. U.S. Environmental Protection Agency. Quality Criteria for Water. EPA 440/9-76-023 (1976).

4. National Academy of Sciences, National Academy of Engineering. Water Quality Criteria 1972. A Report. National Academy of Sciences, Washington, DC. EPA-R3-73-033 (1973).

5. U.S. Public Health Service. Drinking Water Standards. 1962. Title 42, Code of Federal Regulations, Part 72.

6. U.S. Environmental Protection Agency. Water Program. Toxic Pollutant Effluent Standards. Title 40 Code Federal Regulations, Part 129.

7. U.S. Environmental Protection Agency, Office of Toxic Substances. Preliminary Assessment of Suspected Carcinogens in Drinking Water: Report to Congress. Environmental Protection Agency, Washington, DC (1975).

8. Shackelford, W. M., and L. H. Keith. Frequency of Organic Compounds Identified in Water. EPA Publication No. 600/4-76-062, December 1976.

9. Windholz, M., Ed. The Merck Index: An Encyclopedia of Chemicals and Drugs, Ninth Edition. Merck & Co., Inc., Rahway, NJ (1976).

10. Sax, N. I., Ed. Dangerous Properties of Industrial Materials, Fourth Edition. Van Nostrand Reinhold Co., New York, NY (1975).

11. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No . 76-191 (1976).

12. American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values for Substances in Workroom Air with Supplements, Third Edition. American Conference of Governmental Industrial Hygienists, Cincinnati, OH (1974).

218<

CATEGORY 19

HALOGENATED PHENOLIC COMPOUNDS

SUBCATEGORY: 19B - Halogenated Cresols

Summary of Subcategory

Total number of compounds in subcategory	3
number of parent compounds with subspecies	1
number of subspecies	3
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

Consent Decree compounds included in subcategory: 3

19B021	Chlorinated-o-cresol
19B022	Chlorinated-m-cresol
19B023	Chlorinated-p-cresol

CATEGORY: 19B

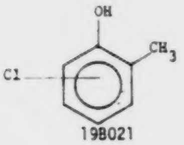
CHLORINATED CRESOLS: C_7H_7ClO (chlorohydroxytoluenes). 19B020
Odorless solids.
CHLORINATED o-CRESOL: A solid. 19B021
CHLORINATED m-CRESOL: A solid. 19B022
CHLORINATED p-CRESOL: A solid. 19B023

PROPERTIES:

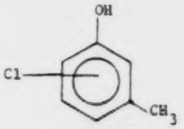
Molecular wt: 142.59; mp: 45-86; bp: 196-228^{760}; soluble to slightly soluble in water.

WLN:

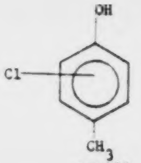
STRUCTURE:



19B021



19B022



19B023

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Chlorinated cresols have been reported in samples taken from river water (ref. 1). Twelve isomeric forms of monochlorinated cresols are possible.

TOXIC PROPERTIES, HEALTH EFFECTS:

Chlorinated cresols are known to be allergens (ref. 2). The introduction of a chlorine group to cresol probably increases toxicity.

LD_{Lo} (oral, rat): 500 mg/kg (ref. 3) for 4-chloro-m-cresol.
Aquatic toxicity: Levels of 0.075 to 0.003 mg/ℓ cause tainting of fish flesh (ref. 4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Chlorinated cresols are on the EPA Consent Decree Priority 3 List.

EPA 1976 Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 5).

NAS/NAE 1972 Water Quality Criteria: 1 μg/l of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/l at any time or place; application factor of 0.05 (ref. 2).

U.S. Public Health Service Drinking Water Standards, 1962--Levels for alternate source selection: 1 μg/l (ref. 6).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$45 \times 500 = 2.25 \times 10^4$ μg/m^3	Air, Ecology:	
Water, Health:	$5 \times 1 = 5$ μg/ℓ	Water, Ecology:	$5 \times 100 = 500$ μg/ℓ
Land, Health:	$0.2 \times 5 = 1$ μg/g	Land, Ecology:	$0.2 \times 500 = 100$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

EPC_{AH2} = 0.107 x 500 = 53.5 μg/m^3
EPC_{AH3} = 0.081 x 500 = 40.5 μg/m^3
EPC_{WH1} = 15 x 40.5 = 608 μg/ℓ
EPC_{WH2} = 0.4 x 500 = 200 μg/ℓ
EPC_{WHS} = 1 μg/ℓ (phenolic compounds)
EPC_{LH} = 0.2 x 1 = 0.2 μg/g

EPC_{WE2} = 3 μg/ℓ (to prevent tainting)
EPC_{WES} = 100 μg/ℓ (phenolic compounds)
EPC_{LE} = 0.2 x 3 = 0.6 μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

19B020
CHLORINATED CRESOLS

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			2.25E4		40.5		
Water, μg/l (ppm Wt)			5.0E0	5.0E2	1	3	
Land, μg/g (ppm Wt)			1.0E0	1.0E2	0.2	0.6	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			40.5		
Water, μg/l (ppm Wt)	1†	100 †	200	3	
Land, μg/g (ppm Wt)			0.2	0.6	

† Phenolic Compounds

REFERENCES: CATEGORY 19B

Halogenated Phenolic Compounds - Halogenated Cresols

1. Shackelford, W. M., and L. H. Keith. Frequency of Organic Compounds Identified in Water. EPA Publication No. 600/4-76-062, December 1976.

2. Sax, N. I., Ed. Dangerous Properties of Industrial Materials, Fourth Edition. Van Nostrand Reinhold Co., New York, NY (1975).

3. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

4. National Academy of Sciences, National Academy of Engineering. Water Quality Criteria 1972. A Report. National Academy of Sciences, Washington, DC. EPA-R3-73-033 (1973).

5. U.S. Environmental Protection Agency. Quality Criteria for Water. EPA 440/9-76-023 (1976).

6. U.S. Public Health Service. Drinking Water Standards. 1962. Title 42, Code of Federal Regulations, Part 72.

CATEGORY 20

NITROPHENOLIC COMPOUNDS

SUBCATEGORY: 20A - Nitrophenols

Summary of Subcategory

Total number of compounds in subcategory	8
number of parent compounds with subspecies	1
number of subspecies	3
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

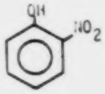
Consent Decree compounds included in subcategory: 3

20A020	2-Nitrophenol
20A060	4-Nitrophenol
20A101	2,4-Dinitrophenol

CATEGORY: 20A

WLN: WNR BQ

STRUCTURE:



2-NITROPHENOL: $C_6H_5NO_3$ (o-nitrophenol, 2-hydroxynitrobenzene). 2-nitrophenol crystallizes as yellow needles from ethanol; peculiar aromatic odor. 20A020

PROPERTIES:

Molecular wt: 139.12; mp: 44.9; bp: 216; d: 1.495; vap. press: 1 mm at 49°; solubility in water: 2,100 mg/ℓ at 20°C; volatile in steam.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

All nitro compounds are potentially explosive.

Nitrophenols are formed by the reaction of nitric acid with phenols. They are used in the synthesis of dyestuffs and other intermediates (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

2-nitrophenol is a stronger acid than phenol. Contact of 2-nitrophenol with the skin may cause irritation or burns. It is absorbed through intact skin and through the respiratory tract (ref. 1). Liver and kidney damage has been observed in experimental animals (ref. 2).

The nitrophenols are methemoglobin formers, but less so than aniline and mononitrobenzene (ref. 1).

Aquatic toxicity: 24-48 hour TLm for bluegill is 46.3 - 67 mg/ℓ (ref. 10).

LD_{50} (oral, rat): 1,297 mg/kg.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 3).

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (for phenols) (ref. 4).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/ℓ (for phenols) (ref. 5).

2-Nitrophenol is on EPA Consent Decree Priority III List.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 1{,}297 = 5.8 \times 10^4$ μg/m^3
Water, Health: $5 \times 1 = 5$ μg/ℓ
Land, Health: $0.2 \times 5 = 1$ μg/g

Air, Ecology:
Water, Ecology: $5 \times 100 = 500$ μg/ℓ
Land, Ecology: $0.2 \times 500 = 100$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 1{,}297 = 139$ μg/m^3
$EPC_{AH3} = 0.081 \times 1{,}297 = 105$ μg/m^3
$EPC_{WH1} = 15 \times 105 = 1{,}580$ μg/ℓ
$EPC_{WH2} = 0.4 \times 1{,}297 = 520$ μg/ℓ
$EPC_{WHS} = 1$ μg/ℓ (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g

$EPC_{WE1} = 50 \times 46 = 230$ μg/ℓ
$EPC_{WES} = 100$ μg/ℓ (phenolic compounds)
$EPC_{LE} = 0.2 \times 100 = 20$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

20A020
2-NITROPHENOL

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			5.8E4		105		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1	100	
Land, $\mu g/g$ (ppm Wt)			1.0E0	1.0E2	0.2	20	

*To be multiplied by dilution factor

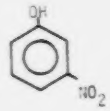
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			105		
Water, $\mu g/l$ (ppm Wt)	1[†]	100[†]	520	230	
Land, $\mu g/g$ (ppm Wt)			0.2	20	

[†] Phenolic compounds.

CATEGORY: 20A

WLN: WNR CQ

STRUCTURE:



3-NITROPHENOL: $C_6H_5NO_3$ (m-nitrophenol). 20A040
3-nitrophenol can be crystallized from an aqueous solution of hydrochloric acid. Colorless to yellow crystals.

PROPERTIES:

Molecular wt: 139.12; mp: 97; bp: 194 at 70 mm; d: 1.485_4^{20}; solubility in water: 13,500 mg/ℓ at 25°C, 133,000 mg/ℓ at 90°C (ref. 10).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

All nitro compounds are potentially explosive.

Nitrophenols are formed by the reaction of nitric acid with phenols. They are used in the synthesis of dyestuffs and other intermediates (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

3-Nitrophenol is a stronger acid than phenol.

Contact of 3-nitrophenol with the skin may cause irritation or burns.

The nitrophenols are methemoglobin formers, but less so than aniline and mononitrobenzene (ref. 1).

LD_{50} (oral, rat): 447 mg/kg.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 3).

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (for phenols) (ref. 4).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/ℓ (for phenols) (ref. 5).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 45 x 447 = 2.0×10^4 μg/m^3
Water, Health: 5 x 1 = 5 μg/ℓ
Land, Health: 0.2 x 5 = 1 μg/g

Air, Ecology:
Water, Ecology: 5 x 100 = 500 μg/ℓ
Land, Ecology: 0.2 x 500 = 100 μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

EPC_{AH2} = 0.107 x 447 = 48 μg/m^3
EPC_{AH3} = 0.081 x 447 = 36 μg/m^3
EPC_{WH1} = 15 x 36 = 540 μg/ℓ
EPC_{WH2} = 0.4 x 447 = 180 μg/ℓ
EPC_{WHS} = 1 μg/ℓ (phenolic compounds)
EPC_{LH} = 0.2 x 1 = 0.2 μg/g

EPC_{WES} = 100 μg/ℓ (phenolic compounds)
EPC_{LE} = 0.2 x 100 = 20 μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

X
20A040
3-NITROPHENOL

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.0E4		36		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1	100	
Land, $\mu g/g$ (ppm Wt)			1.0E 0	1.0E2	0.2	20	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			36		
Water, $\mu g/l$ (ppm Wt)	1 †	100 †	180		
Land, $\mu g/g$ (ppm Wt)			0.2	20	

† Phenolic compounds.

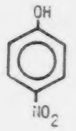
CATEGORY: 20A

WLN: WNR DQ

4-NITROPHENOL: $C_6H_5NO_3$ (p-nitrophenol). 20A060

4-Nitrophenol occurs in two forms: colorless prisms obtained by crystallization from toluene above 63, and yellow crystals obtained by crystallization from toluene below 63. Ordinary 4-nitrophenol is a mixture of both forms; odorless.

STRUCTURE:



PROPERTIES:

Molecular wt: 139.12; mp: 114; bp: 279

d: 1.479^{20}; decomposes at 279; soluble in hot water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

All nitro compounds are potentially explosive.

Nitrophenols are formed by the reaction of nitric acid with phenols. They are used in the synthesis of dyestuffs and other intermediates (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

4-Nitrophenol is a stronger acid than phenol. Contact of 4-nitrophenol with the skin may cause irritation or burns. The biological half-life of 4-nitrophenol in man is reported as 0.041 days (ref. 6). Experiments have shown it to cause central nervous system depression and blood effects (ref. 2).

The nitrophenols are methemoglobin formers, but less so than aniline and mononitrobenzene (ref. 1).

LD_{50} (oral, rat): 350 mg/kg.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 3).

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (for phenols) (ref. 4).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/ℓ (for phenols) (ref. 5)

4-Nitrophenol is on EPA Consent Decree Priority III List.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 350 = 1.6 \times 10^4$ μg/m^3

Water, Health: $5 \times 1 = 5$ μg/ℓ

Land, Health: $0.2 \times 5 = 1$ μg/g

Air, Ecology:

Water, Ecology: $5 \times 100 = 500$ μg/ℓ

Land, Ecology: $0.2 \times 500 = 100$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 350 = 37$ μg/m^3

$EPC_{AH3} = 0.081 \times 350 = 28$ μg/m^3

$EPC_{WH1} = 15 \times 28 = 420$ μg/ℓ

$EPC_{WH2} = 0.4 \times 350 = 140$ μg/ℓ

$EPC_{WHS} = 1$ μg/ℓ (phenolic compounds)

$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g

$EPC_{WES} = 100$ μg/ℓ (phenolic compounds)

$EPC_{LE} = 0.2 \times 100 = 20$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

X
20A060
4-NITROPHENOL

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, µg/m³ (ppm Vol)			1.6E4		28		
Water, µg/l (ppm Wt)			5.0E0	5.0E2	1	100	
Land, µg/g (ppm Wt)			1.0E 0	1.0E2	0.2	20	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, µg/m³ (ppm Vol)			28		
Water, µg/l (ppm Wt)	1†	100†	140		
Land, µg/g (ppm Wt)			0.2	20	

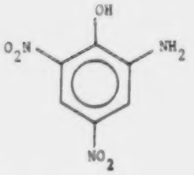
† Phenolic compounds.

CATEGORY: 20A

WLN:

2-AMINO-4,6-DINITROPHENOL: $C_6H_5N_3O_5$
(picramic acid, picraminic acid, dinitroaminophenol). 20A080
A solid. Dark red needles from alcohol, prisms from chloroform.

STRUCTURE:



PROPERTIES:
Molecular wt: 199.12; mp: 169; flashes at 210; slightly soluble in water, 65 mg/100 mℓ at 22-25°C.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

2-Amino-4,6-dinitrophenol is used in the manufacture of azo dyes, as an acid-base indicator, and as a reagent for albumin (ref. 1).

It has been identified in samples of finished drinking water (ref. 11).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological characteristics of 2-amino-4,6-dinitrophenol are reported to be similar to 2,4-dinitrophenol (ref. 7). Toxicological data concerning dinitrophenols are given below.

Dinitrophenols are stronger acids than phenol. Contact of dinitrophenols with the skin may cause irritation or burns; they are readily absorbed through intact skin and through the respiratory tract (ref. 7). Ingestion of 36 mg/kg of 2,4-dinitrophenol has resulted in human death (ref. 8).

Animal experiments indicate that dinitrophenols are more toxic than nitrophenols. They can cause increases in metabolism and temperature, dermatitis, and eye and nerve damage (ref. 7).

LD_{50} (oral, rat): 30 mg/kg for 2,4-dinitrophenol (ref. 8).

Aquatic toxicity: 96 hr TLm for 2,4-dinitrophenol is 10-1 ppm (ref. 8).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/l of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 3).

NAS/NAE 1972 Water Quality Criteria: 1 μg/l of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/l at any time or place; application factor of 0.05 (for phenols) (ref. 4).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/l (for phenols) (ref. 5).

2,4-dinitrophenol is on EPA Consent Decree Priority III List.

* **MINIMUM ACUTE TOXICITY CONCENTRATIONS**:

Air, Health: $45 \times 30 = 1.35 \times 10^3$ μg/m^3	Air, Ecology:
Water, Health: $5 \times 1 = 5$ μg/l	Water, Ecology: $100 \times 1 = 100$ μg/ℓ
Land, Health: $0.2 \times 5 = 1.0$ μg/g	Land, Ecology: $0.2 \times 100 = 20$ μg/g

* **ESTIMATED PERMISSIBLE CONCENTRATIONS**:

$EPC_{AH2} = 0.107 \times 30 = 3.2$ μg/m^3	
$EPC_{AH3} = 0.081 \times 30 = 2.4$ μg/m^3	
$EPC_{WH1} = 15 \times 2.4 = 36$ μg/l	$EPC_{WE1} = 50 \times 1 = 50$ μg/l
$EPC_{WH2} = 0.4 \times 30 = 12$ μg/l	
$EPC_{WHS} = 1$ μg/l (phenolic compounds)	$EPC_{WES} = 100$ μg/l (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g	$EPC_{LE} = 0.2 \times 50 = 10$ μg/g

*Based on data for 2,4-dinitrophenol.

MULTIMEDIA ENVIRONMENTAL GOALS

X
20A080
2-AMINO-4,6-DINITROPHENOL

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			1.35E3		2.4		
Water, μg/l (ppm Wt)			5.0E0	1.0E2	1	50	
Land, μg/g (ppm Wt)			1.0E0	2.0E1	0.2	10	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			2.4		
Water, μg/l (ppm Wt)	1†	100†	12	50	
Land, μg/g (ppm Wt)			0.2	10	

†Phenolic Compound

CATEGORY: 20A

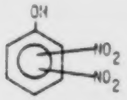
WLN: WNR XQ XNW

DINITROPHENOLS: $C_6H_4N_2O_5$ (dinitrohydroxybenzenes). 20A100

Dinitrophenols crystallize as colorless or yellowish crystals.

2,4-DINITROPHENOL: 20A101
2,5-DINITROPHENOL: 20A102
2,6-DINITROPHENOL: 20A103

STRUCTURE:



PROPERTIES:

	Mol.wt.	mp	bp	d	solubility	vap.d.
2,4-dinitrophenol	184.11	115	sublimes	1.683	slightly sol.	6.35
2,5-dinitrophenol	184.11	108	-	-	slightly sol.	-
2,6-dinitrophenol	184.11	63	-	-	insol.	6.35
All isomers		63-144	-	1.672-1.702	-	-

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

All nitro compounds are potentially explosive.

Nitrophenols are formed by the reaction of nitric acid with phenols.

The dinitrophenols are used as a mixture in the synthesis of dyestuffs and picric and picramic acids. They are used in the preservation of timber and in the manufacture of a photographic developer (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

Dinitrophenols are stronger acids than phenol. Contact of dinitrophenols with the skin may cause irritation or burns; they are readily absorbed through intact skin and through the respiratory tract (ref. 7). Ingestion of 36 mg/kg of 2,4-dinitrophenol has resulted in human death (ref. 8).

Animal experiments indicate that dinitropnenols are more toxic than nitrophenols. They can cause increases in metabolism and temperature, dermatitis, and eye and nerve damage (ref. 7).

LD_{Lo} (oral, rat): 30 mg/kg for dinitrophenol (presumably this is for a mixture of the various isomers.)

The lowest LD_{50} (oral, rat) for a single dinitrophenol isomer is reported as 30 mg/kg for 2,4-dinitrophenol.

Aquatic toxicity: 96-hour TLm for 2,4-dinitrophenol is 10-1 ppm (ref. 8).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

EPA 1976 Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 3).

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (for phenols) (ref. 4).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/ℓ (for phenols) (ref. 5).

2,4-dinitrophenol is on EPA Consent Decree Priority III List.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 30 = 1.35 \times 10^3$ μg/m³
Water, Health: $5 \times 1 = 5$ μg/ℓ
Land, Health: $0.2 \times 5 = 1$ μg/g

Air, Ecology:
Water, Ecology: $100 \times 1 = 100$ μg/ℓ
Land, Ecology: $0.2 \times 100 = 20$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 30 = 3.2$ μg/m³
$EPC_{AH3} = 0.081 \times 30 = 2.4$ μg/m³
$EPC_{WH1} = 15 \times 2.4 = 36$ μg/ℓ
$EPC_{WH2} = 0.4 \times 30 = 12$ μg/ℓ
$EPC_{WHS} = 1$ μg/ℓ (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g

$EPC_{WE1} = 50 \times 1 = 50$ μg/ℓ
$EPC_{WES} = 100$ μg/ℓ (phenolic compounds)
$EPC_{LE} = 0.2 \times 50 = 10$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

X
20A100
DINITROPHENOLS

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.35E3		2.4		
Water, $\mu g/l$ (ppm Wt)			5.0E0	1.0E2	1	50	
Land, $\mu g/g$ (ppm Wt)			1.0E 0	2.0E1	0.2	10	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			2.4		
Water, $\mu g/l$ (ppm Wt)	$1^{\dagger}$	$100^{\dagger}$	12	50	
Land, $\mu g/g$ (ppm Wt)			0.2	10	

† Phenolic compounds.

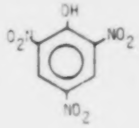
233<

CATEGORY: 20A

WLN: WNR BQ CNW ENW

2,4,6-TRINITROPHENOL: $C_6H_3N_2O_7$ (picric acid).
Yellow crystals; odorless. 20A120

STRUCTURE:



PROPERTIES:

Molecular wt: 229.11; mp: 121.8; explodes above 300°; d: 1.763; vap. d: 7.90; slightly soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Picric acid is a hazardous chemical. It is a known explosive. It reacts with metals to form picrates, which are also explosive.

Nitrophenols are formed by the reaction of nitric acid with phenols.

TOXIC PROPERTIES, HEALTH EFFECTS:

Picric acid is a strong acid ($K_A \approx 10^{-1}$).

Contact of picric acid with the skin may cause irritation, burns, or allergic reactions (ref. 7).

Picric acid is absorbed through the skin. Ingestion of 1 to 2 grams in man causes severe poisoning (ref. 9).

LD_{Lo} (unknown route of administration, dog): 60 mg/kg.

LD_{Lo} (oral, rabbit): 120 mg/kg.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.1 mg/m^3 (0.01 ppm).

EPA 1976 Water Quality Criteria : 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 3).

NAS/NAE 1972 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (for phenols) (ref. 4).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/ℓ (for phenols) (ref. 5).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 100 μg/m^3 (0.011 ppm)
Water, Health: 5 x 1 = 5 μg/ℓ
Land, Health: 0.2 x 5 = 1 μg/g

Air, Ecology:
Water, Ecology: 5 x 100 = 500 μg/ℓ
Land, Ecology: 0.2 x 500 = 100 μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 0.1/420 = 0.24$ μg/m^3
$EPC_{AH1a} = 0.011/420 = 2.6 \times 10^{-5}$ ppm
$EPC_{WH1} = 15 \times 0.24 = 3.6$ μg/ℓ
$EPC_{WH2} = 13.8 \times 0.1 = 1.4$ μg/ℓ
$EPC_{WHS} = 1$ μg/ℓ (phenolic compounds)
$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g

$EPC_{WES} = 100$ μg/ℓ (phenolic compounds)
$EPC_{LE} = 0.2 \times 100 = 20$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

XX
20A120
2,4,6-TRINITROPHENOL

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.0E2 (0.011)		0.24 (0.00003)		
Water, μg/l (ppm Wt)			5.0E0	5.0E2	1	100	
Land, μg/g (ppm Wt)			1.0E 0	1.0E2	0.2	20	

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			0.24 (0.00003)		
Water, μg/l (ppm Wt)	1 †	100†	1.4		
Land, μg/g (ppm Wt)			0.2	20	

† Phenolic compounds.

REFERENCES: CATEGORY 20A

Nitrophenolic Compounds - Nitrophenols

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CATEGORY 20

NITROPHENOLIC COMPOUNDS

SUBCATEGORY: 20B - Nitrocresols

Summary of Subcategory

Total number of compounds in subcategory	3
number of parent compounds with subspecies	1
number of subspecies	2
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

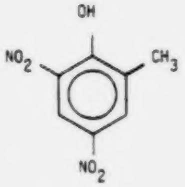
Consent Decree compounds included in subcategory: None

CATEGORY: 20B

4,6-DINITRO-o-CRESOL: $C_7H_6N_2O_5$ (2,4-dinitro-o-cresol, 2-methyl-4,6-dinitrophenol, 3,5-dinitro-2-hydroxy toluene). Crystallizes as yellow prisms from ethanol. 20B020.

WLN: WNR BQ C ENW

STRUCTURE:



PROPERTIES:

Molecular wt: 198; mp: 87.5; sparingly soluble in water; vap. d: 6.82; moderately volatile with steam.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

All nitro compounds are potentially explosive.

Nitrophenols are formed by the reaction of nitric acid with phenols.

4,6-Dinitro-o-cresol is a selective herbicide and insecticide (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

4,6-Dinitro-o-cresol is a stronger acid than cresol. Contact with the skin may cause irritation or burns. Local necrosis and dangerous systemic effects may result (ref. 1). Toxicity resembles that of dinitrophenol (ref. 2).

Inhalation of 1 mg/m^3 has produced central nervous system effects in man (ref. 3). Repeated daily exposure results in considerable accumulation (ref. 4). The biological half-life in man is reported to be 5.78 days (ref. 5).

LD_{50} (oral, rat): 25 mg/kg (ref. 3).

LC_{Lo} (inhalation, cat): 40 mg/m^3 (ref. 3).

Aquatic toxicity: TLm 96: 10-1 ppm (ref. 3).

The compound is very phytotoxic (ref. 6).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

4,6-Dinitro-o-cresol is on EPA Consent Decree Priority III List.

TLV = 0.2 mg/m^3 (0.025 ppm)

EPA Water Quality Criteria: 1 μg/ℓ of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 7).

NAS/NAE 1976 Water Quality Criteria: 1 μg/ℓ of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/ℓ at any time or place; application factor of 0.05 (for phenols)(ref. 8).

U.S. Public Health Service Drinking Water Regulations, 1962--Levels for alternate source selection: 1 μg/ℓ (for phenols)(ref. 9).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 200 μg/m^3 (0.025 ppm)

Water, Health: 5 x 1 = 5 μg/ℓ

Land, Health: 0.2 x 5 = 1 μg/g

Air, Ecology:

Water, Ecology: 5 x 100 = 500 μg/ℓ

Land, Ecology: 0.2 x 500 = 100 μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 0.2/420 = 0.5$ μg/m^3

$EPC_{AH1a} = 0.025/420 = 6 \times 10^{-5}$ ppm

$EPC_{WH1} = 15 \times 0.5 = 7.5$ μg/ℓ

$EPC_{WH2} = 13.8 \times 0.2 = 3$ μg/ℓ

$EPC_{WHS} = 1$ μg/ℓ (phenolic compounds)

$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g

$EPC_{WE1} = 50 \times 1 = 50$ μg/ℓ

$EPC_{WES} = 100$ μg/ℓ (phenolic compounds)

$EPC_{LE} = 0.2 \times 50 = 10$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

XX
20B020
4,6-DINITRO-o-CRESOL

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.0E2 (0.025)		0.5 (6×10^{-5})		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1	50	
Land, $\mu g/g$ (ppm Wt)			1.0E0	1.0E2	0.2	10	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			0.5 (6×10^{-5})		
Water, $\mu g/l$ (ppm Wt)	1†	100†	3	50	
Land, $\mu g/g$ (ppm Wt)			0.2	10	

† Phenolic compounds.

CATEGORY: 20B

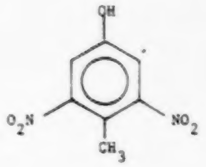
DINITRO-p-CRESOLS: $C_7H_6N_2O_5$ 20B040

3,5-DINITRO-P-CRESOL: Solid crystals. 20B041

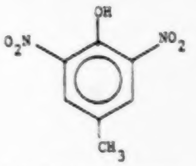
2,6-DINITRO-P-CRESOL: Solid crystals. 20B042

WLN:

STRUCTURE:



3,5-dinitro-p-cresol



2,6-dinitro-p-cresol

PROPERTIES:

	mol.wt.	mp	solubility in water
3,5-dinitro-p-cresol	198.1		
2,6-dinitro-p-cresol	198.1	85	slightly

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

2,6-Dinitro-p-cresol is used in dyestuff synthesis and in the manufacture of photographic developer (ref. 6).

All nitro compounds are potentially explosive.

Nitrophenols are formed by the reaction of nitric acid with phenols.

TOXIC PROPERTIES, HEALTH EFFECTS:

3,5-Dinitro-p-cresol may cause brain damage, as well as damage to the liver and kidneys (ref.6).

Chemical	LD_{50} (mg/kg)	LD_{Lo} (mg/kg)
3,5-dinitro-p-cresol		15 (unknown route of administration, dog)
2,6-dinitro-p-cresol	24.8 (intraperitoneal, mouse)	

Toxicity is similar to that of 4,6-dinitro-o-cresol (ref. 2).

Aquatic toxicity: TLm 96:10-1 ppm for 4,6-dinitro-o-cresol (ref. 3).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (0.025 ppm) for 4,6-dinitro-o-cresol.

EPA 1976 Water Quality Criteria: 1 μg/l of phenol (including phenolic compounds) for domestic water supply (welfare) and to protect against fish flesh tainting (ref. 3).

NAS/NAE 1972 Water Quality Criteria: 1 μg/l of phenolic compounds in public water supply sources to prevent odor from chlorinated phenols. To prevent tainting and toxic effects in aquatic life: Concentration no greater than 100 μg/l at any time or place; application factor of 0.05 (ref. 4).

U.S. Public Health Service Drinking Water Standards, 1962--Levels for alternate source selection: 1 μg/l (ref. 5).

***MINIMUM ACUTE TOXICITY CONCENTRATIONS**:

Air, Health: 200 μg/m^3 (0.025 ppm)

Water, Health: 5 x 1 = 5 μg/ℓ

Land, Health: 0.2 x 5 = 1 μg/g

Air, Ecology:

Water, Ecology: 5 x 100 = 500 μg/ℓ

Land, Ecology: 0.2 x 500 = 100 μg/g

***ESTIMATED PERMISSIBLE CONCENTRATIONS**:

$EPC_{AH1} = 10^3 \times 0.2/420 = 0.5$ μg/m^3

$EPC_{AH1a} = 0.025/420 = 6 \times 10^{-5}$ ppm

$EPC_{WH1} = 15 \times 0.5 = 7.5$ μg/ℓ

$EPC_{WH2} = 13.8 \times 0.2 = 3$ μg/ℓ

$EPC_{WHS} = 1$ μg/l (phenolic compounds)

$EPC_{LH} = 0.2 \times 1 = 0.2$ μg/g

$EPC_{WE1} = 50 \times 1 = 50$ μg/l

$EPC_{WES} = 100$ μg/l (phenolic compounds)

$EPC_{LE} = 0.2 \times 50 = 10$ μg/g

*Based on data for 4,6-dinitro-o-cresol.

XX
20B040
DINITRO-p-CRESOLS

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors †				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.0E2 (0.025)		0.5 (6×10^{-5})		
Water, $\mu g/l$ (ppm Wt)			5.0E0	5.0E2	1	50	
Land, $\mu g/g$ (ppm Wt)			1.0E0	1.0E2	0.2	10	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			0.5 (6×10^{-5})		
Water, $\mu g/l$ (ppm Wt)	1‡	100‡	3	50	
Land, $\mu g/g$ (ppm Wt)			0.2	10	

† Based on data for 4,6-dinitro-o-cresol

‡ Phenolic compounds.

REFERENCES: CATEGORY 20B

Nitrophenolic Compounds - Nitrocresols

1. Windholz, M., Ed. The Merck Index: An Encyclopedia of Chemicals and Drugs, Ninth Edition. Merck and Co., Inc., Rahway, NJ (1976).

2. Hamblin, D. O. Aromatic Nitro and Amino Compounds. Industrial Hygiene and Toxicology, Second Revised Edition, Vol. 2, Interscience Publishers, New York, NY (1963).

3. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco, Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication (NIOSH) No. 76-191 (1976).

4. American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values for Substances in Workroom Air with Supplements, Third Edition. American Conference of Governmental Industrial Hygienists, Cincinnati, OH (1974).

5. Handy, R., and A. Schindler. Estimation of Permissible Concentration of Pollutants for Continuous Exposure. Prepared by Research Triangle Institute under Contract 68-02-1325 for Environmental Protection Agency, Research Triangle Park, NC, EPA-600 12-76-155 (1976).

6. Sax, N. I., Ed. Dangerous Properties of Industrial Materials, Fourth Edition. Van Nostrand Reinhold Co., New York, NY (1975).

7. U.S. Environmental Protection Agency. Quality Criteria for Water. EPA 440/9-76-023 (1976).

8. National Academy of Sciences, National Academy of Engineering. Water Quality Criteria 1972. National Academy of Sciences, Washington, DC. EPA-R3-73-033 (1973).

9. U.S. Public Health Service. Drinking Water Standards: 1972. Title 42, Code of Federal Regulations, Part 72.

CATEGORY 21

FUSED POLYCYCLIC HYDROCARBONS

SUBCATEGORY: 21A - Two- and Three-Ring Fused Polycyclic Hydrocarbons

Summary of Subcategory

Total number of compounds in subcategory	17
number of parent compounds with subspecies	4
number of subspecies	11
Number of parent compounds with no MEG values	4
Number of parent compounds with natural background levels only	1
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	3

Consent Decree compounds included in subcategory: 4

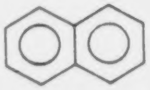
21A020	Naphthalene
21A100	Acenapthene
21A140	Anthracene
21A180	Phenanthrene

CATEGORY: 21A

WLN: L66J

NAPHTHALENE: $C_{10}H_8$ (naphthalin, naphthaline, naphthene, tar camphor). 21A020.
Colorless monoclinic crystals, aromatic odor.

STRUCTURE:



PROPERTIES:

Molecular wt: 128.18 mp: 80.55, bp: 218, 87.5^{10}; d: 1.0253^{20}, 0.9625_4^{1000}; vap. press: 1 mm at 52.6° C; vap.d: 4.42; very low solubility in water; 3 mg/100 mℓ solubility may be enhanced by surfactant impurities in water (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Naphthalene is among the lower molecular weight polycyclic hydrocarbons comprising the volatile portion of the benzene-soluble fraction of coal tar (ref. 2). Concentrations of 3.8 to 11.2 μg/m³ in urban air are reported (ref. 3). Naphthalene is associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 4). The following concentrations of PPAH have been estimated or reported: Air (urban environment in winter in seven selected U.S. cities): 21.6 ng/m³ - 146 ng/m³ (ref. 4); groundwater and surface treated water: 0.001 μg/ℓ - 0.025 μg/ℓ (ref. 1); upper layer of Earth's crust: 100 μg/kg - 1,000 μg/kg (ref. 1).

Naphthalene is a byproduct of the coke industry and is recovered from coal tar (ref. 15). It is also produced in petroleum refining (ref. 16). It is used as a moth repellant, in chemical and dye manufacturing, in preserving wood, and in other uses (ref. 15).

Odor threshold is reported as 0.004 and 0.140 (ref. 16).

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{50} (oral, rat): 1,780 mg/kg.

Naphthalene may cause irritation in concentrations of 15 ppm, and serious damage to eyes may result from continuous exposure (ref. 2). It is readily absorbed when inhaled (ref. 15).

Naphthalene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 5). Naphthalene is reported to cause tumors in rats. The EPA/NIOSH ordering number is 4101. The lowest dose to induce an oncogenic response is reported as 3,500 mg/kg. The adjusted ordering number is 1.17. Naphthalene is considered inactive as a carcinogen (ref. 5).

Naphthalene has been rated as moderately toxic to aquatic organisms. The 96-hour TLm is reported as 1-10 ppm (ref. 6). Naphthalene in concentrations of 1 mg/ℓ may cause tainting of fish flesh (refs. 7,8).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Naphthalene appears on EPA Consent Decree List with an assigned priority of 2.

TLV: 50 mg/m³ (10 ppm)

TLV for coal-tar pitch: 0.2 mg/m³ [The specification includes naphthalene, anthracene, acridine, phenanthrene, and fluorene collectively. The purpose of the TLV is to minimize concentrations of higher weight polycyclic hydrocarbons which are carcinogenic (ref. 2).]

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 5.0×10^4 μg/m³ (10 ppm)
Water, Health: $15 \times 5.0 \times 10^4 = 7.5 \times 10^5$ μg/ℓ
Land, Health: $0.2 \times 7.5 \times 10^5 = 1.5 \times 10^5$ μg/g

Air, Ecology:
Water, Ecology: $100 \times 1 = 100$ μg/ℓ
Land, Ecology: $0.2 \times 100 = 20$ μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 50/420 = 119$ μg/m³
$EPC_{AH1a} = 10/420 = 0.02$ ppm
$EPC_{WH1} = 15 \times 119 = 1,785$ μg/ℓ
$EPC_{WH2} = 13.8 \times 50 = 690$ μg/ℓ
$EPC_{LH} = 0.2 \times 690 = 138$ μg/g
$EPC_{AC2} = 10^3/(6 \times 1.17) = 142$ μg/m³
$EPC_{WC} = 15 \times 142 = 2,130$ μg/ℓ
$EPC_{LC} = 0.2 \times 2,130 = 426$ μg/g

$EPC_{WE1} = 50 \times 1 = 50$ μg/ℓ
$EPC_{WE2} = 1,000$ μg/ℓ (to prevent tainting)
$EPC_{LE} = 0.2 \times 50 = 10$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

21A020
NAPHTHALENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			5.0E4 (10)		119 (0.02)		3.8 to 11.2†
Water, μg/l (ppm Wt)			7.5E5	1.0E2	690	50	
Land, μg/g (ppm Wt)			1.5E5	2.0E1	138	10	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			119 (0.02)		142
Water, μg/l (ppm Wt)			690	50	2,130
Land, μg/g (ppm Wt)			138	10	426

† Reported for urban atmosphere. No rural concentration is required.

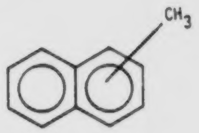
CATEGORY: 21A

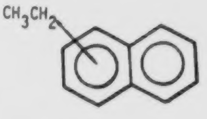
WLN:

MONOALKYL NAPHTHALENES: 21A040

1-METHYLNAPHTHALENE:	$C_{11}H_{10}$.	A colorless liquid. 21A041
2-METHYLNAPHTHALENE:	$C_{11}H_{10}$.	A solid. 21A042
1-ETHYLNAPHTHALENE:	$C_{12}H_{12}$.	A liquid. 21A043
2-ETHYLNAPHTHALENE:	$C_{12}H_{12}$.	A liquid. 21A044

STRUCTURE:





PROPERTIES:

	mol.wt.	mp.	bp.	d.	solubility in water
1-methylnaphthalene	142.20	-32	240-3	1.025	insoluble
2-methylnaphthalene	142.20	34	241-2	0.994	insoluble
1-ethylnaphthalene	156.23	-13.88	258.7^{760}	1.6062^{20}	insoluble
2-ethylnaphthalene	156.23	-7.4	257.9^{760}	1.5999^{20}	insoluble

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

1-Methylnaphthalene and 2-methylnaphthalene have been reported in samples taken from finished drinking water. 2-Methylnaphthalene has also been reported in samples taken from lake water (ref. 9).

Monoalkyl naphthalenes are likely to be associated with coal-tar and with particulate polycyclic aromatic hydrocarbons.

1-Methyl naphthalene is produced in petroleum refining and in coal processing. It is a constituent of asphalt and of naphtha (ref. 16). It is used in organic synthesis and in insecticide manufacturing (ref. 16).

The odor of the methyl naphthalenes is detectable in water by 20% of the population at levels of 2 μg/ℓ (ref. 16).

TOXIC PROPERTIES, HEALTH EFFECTS:

Specific toxic effects are not reported but are probably similar to those of naphthalenes.

LD_{Lo} (oral, rat): 5,000 mg/kg for 1-methyl naphthalene, 2-methyl naphthalene, 1 ethyl naphthalene, and 2-ethyl naphthalene (ref. 6).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m³ (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$45 \times 5{,}000 = 2.25 \times 10^5$ μg/m³	Air, Ecology:
Water, Health:	$15 \times 2.25 \times 10^5 = 3.38 \times 10^6$ μg/l	Water, Ecology:
Land, Health:	$0.2 \times 3.38 \times 10^6 = 6.76 \times 10^5$ μg/g	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 5{,}000 = 535$ μg/m³

$EPC_{AH3} = 0.081 \times 5{,}000 = 405$ μg/m³

$EPC_{WH1} = 15 \times 405 = 6{,}075$ μg/l

$EPC_{WH2} = 0.4 \times 5{,}000 = 2{,}000$ μg/l

$EPC_{LH} = 0.2 \times 2{,}000 = 400$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

21A040
MONOALKYL NAPHTHALENES

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.25E5		405		
Water, $\mu g/l$ (ppm Wt)			3.38E6		2,000		
Land, $\mu g/g$ (ppm Wt)			6.76E5		400		

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			405		
Water, $\mu g/l$ (ppm Wt)			2,000		
Land, $\mu g/g$ (ppm Wt)			400		

CATEGORY: 21A

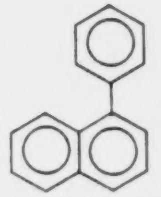
PHENYLNAPHTHALENES: $C_{10}H_7C_6H_5$ 21A060

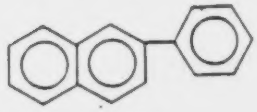
1-PHENYLNAPHTHALENE: A waxy solid. 21A061

2-PHENYLNAPHTHALENE: A solid. 21A062

WLN:

STRUCTURE:


1-phenylnaphthalene


2-phenylnaphthalene

PROPERTIES:

	mol.wt.	mp.	bp.	d.	solubility in water
1-phenylnaphthalene:	204.28	45	334^{760}	1.096_4^{20}	insoluble
2-phenylnaphthalene:	204.28	103-4	345-6	--	--

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

It has been reported that 1,4-diphenylbuta-1,3-dienes, without nitro substituents, undergo photo-reaction and oxidation to 1-phenylnaphthalene (ref. 17).

Phenylnaphthalenes are likely to be associated with particulate polycyclic aromatic hydrocarbons.

TOXIC PROPERTIES, HEALTH EFFECTS:

Certain polycyclic aromatic hydrocarbons, when administered topically to animals, may induce tumors at the site of application (ref. 5).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m³ (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

21A060
PHENYLNAPHTHALENES

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
Category	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

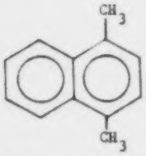
CATEGORY: 21A

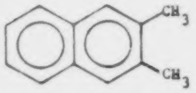
DIMETHYLNAPHTHALENES: $C_{10}H_6C_2H_6$ 21A080

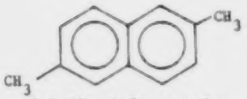
1,4-DIMETHYLNAPHTHALENE: (α-dimethylnaphthalene). A liquid. 21A081
2,3-DIMETHYLNAPHTHALENE: (guaiene). A solid. 21A082
2,6-DIMETHYLNAPHTHALENE: A solid. 21A083

WLN:

STRUCTURE:


1,4-dimethylnaphthalene


2,3-dimethylnaphthalene


2,6-dimethylnaphthalene

PROPERTIES:

	mol.wt.	mp.	bp.	d.	solubility in water
1,4-dimethylnaphthalene	156.23	7.66	268^{760}	1.0166^{20}_{4}	insoluble
2,3-dimethylnaphthalene	156.23	105	268^{760}	1.003^{20}_{4}	insoluble
2,6-dimethylnaphthalene	156.23	110-1	$261\text{-}2^{760}$	1.142^{0}_{4}	insoluble

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Dimethylnaphthalenes have been isolated from crude petroleum oil (ref. 5) and from coal tar (ref. 16).

Dimethylnaphthalenes have been reported in samples taken from finished drinking water and from river water (ref. 9).

Dimethylnaphthalenes are likely to be associated with particulate polycyclic aromatic hydrocarbons.

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{Lo} (oral,rat): 5,000 mg/kg for 1,6-dimethylnaphthalene (ref. 6).

Specific toxic properties are not reported. Toxicity is probably similar to that of monoalkyl naphthalenes and naphthalene.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m³ (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$45 \times 5{,}000 = 2.25 \times 10^5$ μg/m³	Air, Ecology:
Water, Health:	$15 \times 2.25 \times 10^5 = 3.38 \times 10^6$ μg/l	Water, Ecology:
Land, Health:	$0.2 \times 3.38 \times 10^6 = 6.76 \times 10^5$ μg/g	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 5{,}000 = 535$ μg/m³
$EPC_{AH3} = 0.081 \times 5{,}000 = 405$ μg/m³
$EPC_{WH1} = 15 \times 405 = 6{,}075$ μg/l
$EPC_{WH2} = 0.4 \times 5{,}000 = 2{,}000$ μg/l
$EPC_{LH} = 0.2 \times 2{,}000 = 400$ μg/g

21A080
DIMETHYLNAPHTHALENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.25E5		405		
Water, $\mu g/l$ (ppm Wt)			3.38E6		2,000		
Land, $\mu g/g$ (ppm Wt)			6.76E5		400		

*To be multiplied by dilution factor

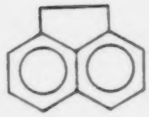
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			405		
Water, $\mu g/l$ (ppm Wt)			2,000		
Land, $\mu g/g$ (ppm Wt)			400		

CATEGORY: 21A

ACENAPHTHENE: $C_{10}H_6(CH_2)_2$ (1,2-dihydroacenaphthylene, periethylenenaphthalene, 1,8-ethylenenaphthalene, naphthyleneethylene). 21A100
White elongate crystals.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt:154.21; mp:96.2; bp:279^{760}; d:1.0242^{99}_{4}; vap. press: 10 mm at 131.2°; vap.d:5.32; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Acenaphthene is found to occur naturally in coal tar and in petroleum residues (ref. 10) and is likely to be associated with particulate polycyclic aromatic hydrocarbons.

Acenaphthene is used as a dye intermediate, in the manufacture of plastics, and as an insecticide and a fungicide. It can be formed by the heated reaction between ethylene and benzene or naphthalene (ref. 10).

Acenaphthene has been found in samples taken from finished drinking water, well water, and river water (ref. 9) and in urban air (ref. 11).

TOXIC PROPERTIES, HEALTH EFFECTS:

Acenaphthene is irritating to the skin and mucous membranes (ref. 12).

Certain polycyclic aromatic hydrocarbons, when administered topically to animals, may induce tumors at the site of application (ref. 5).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Acenaphthene is on the EPA Consent Decree Priority 1 list.

TLV (coal tar pitch volatiles): 0.2 mg/m³.

(The specification includes naphthalene, anthracene, acridine, phenanthrene, and fluorene, collectively. The purpose of the TLV is to minimize concentrations of higher weight polycyclic hydrocarbons that are carcinogenic [ref. 2].)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

21A100
ACENAPHTHENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

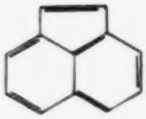
*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

CATEGORY: 21A
ACENAPHTHYLENE: $C_{10}H_6(CH)_2$ 21A120
A solid.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt:152.21; mp:92-3; bp:265-75; d:0.8988^{16}_{2}; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Acenaphthylene has been reported in samples taken from finished drinking water and from well water (ref. 9).

Acenaphthylene is likely to be associated with particulate polycyclic aromatic hydrocarbons.

TOXIC PROPERTIES, HEALTH EFFECTS:

Certain poylycyclic aromatic hydrocarbons, when administered topically to animals, may induce tumors at the site of application (ref. 5).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV (coal tar pitch volatiles): 0.2 mg/m^3

(The specification includes naphthalene, anthracene, acridine, phenanthrene, and fluorene, collectively. The purpose of the TLV is to minimize concentrations of higher weight polycyclic hydrocarbons that are carcinogenic [ref. 2]).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

21A120
ACENAPHTHYLENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

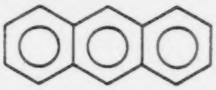
CATEGORY: 21A

WLN: L C666J

ANTHRACENE: $C_{14}H_{10}$

Colorless, monoclinic plates (when pure) with violet fluorescence. 21A140

STRUCTURE:



PROPERTIES:

Molecular wt: 178; mp: 216.2-216.4; bp: 340, 226.5^{53}; d: 1.283^{25}; vap.press.: 1 mm at 145.0° C; sublimes; vap. d: 6.15; insoluble in water, solubility may be enhanced by surfactant impurities in water (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Anthracene is among the lower molecular weight polycyclic hydrocarbons comprising the volatile portion of the benzene-soluble fraction of coal tar (ref. 2). Concentrations of 0.5252 μg/1,500 m^3 and 2 μg/1,000 m^3 in urban air are reported (ref. 3). This is equivalent to 0.00035 to 0.002 μg/m^3. Anthracene is associated with particulate polycyclic aromatic hydrocarbons, PPAH, (ref. 4). The following concentrations of PPAH have been estimated or reported: Air (urban environment in winter in seven selected U.S. cities): 21.6 ng/m^3 - 146 ng/m^3 (ref. 4); ground-water and surface-treated water: 0.001 μg/ℓ - 0.025 μg/ℓ (ref. 1); upper layer of Earth's crust: 100 μg/kg - 1,000 μg/kg (ref. 1); upper layer of Earth's crust: 100 μg/kg - 1,000 μg/kg (ref. 1); estuarine sediment: 8 μg/kg - 170 μg/kg (ref. 11).

Anthracene is an important source of dyestuffs (ref. 10).

TOXIC PROPERTIES, HEALTH EFFECTS:

No specific information is available relative to acute toxic properties of anthracene. Anthracene may be present in soot, coal-tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 5). Anthracene has been shown to produce tumors in mice. The EPA/NIOSH ordering number is 4112. The lowest dose to induce an oncogenic response is reported as 3,300 mg/kg. The adjusted ordering number is 1.25.

Anthracene is considered inactive as a carcinogen (ref. 5).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Anthracene appears on EPA Consent Decree List with an assigned priority of 1. TLV (coal tar pitch volatiles): 0.2 mg/m^3. [The specification includes naphthalene, anthracene, acridine, phenathrene, and fluorene, collectively. The purpose of the TLV is to minimize concentrations of higher-weight polycyclic hydrocarbons which are carcinogenic (ref. 2).]

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/1.25 = 5.6 \times 10^4$ μg/m^3

Water, Health: $15 \times 5.6 \times 10^4 = 8.4 \times 10^5$ μg/ℓ

Land, Health: $0.2 \times 8.4 \times 10^5 = 1.68 \times 10^5$ μg/g

Air, Ecology:

Water, Ecology:

Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 1.25) = 133$ μg/m^3

$EPC_{WC} = 15 \times 133 = 1{,}995$ μg/ℓ

$EPC_{LC} = 0.2 \times 1{,}995 = 399$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

21A140
ANTHRACENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			5.6E4		133		0.00035- 0.002+
Water, μg/l (ppm Wt)			8.4E5		1,995		
Land, μg/g (ppm Wt)			1.7E5		399		

*To be multiplied by dilution factor

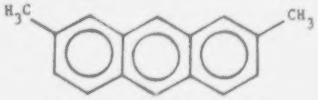
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)					133
Water, μg/l (ppm Wt)					1,995
Land, μg/g (ppm Wt)					399

+ Reported For Urban Atmosphere. No Rural Concentration Is Reported.

CATEGORY: 21A
2,7-DIMETHYLANTHRACENE: $C_{16}H_{14}$ 21A160
Yellow crystals.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 206.112; mp: 241, insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

2,7-Dimethylanthracene is likely to be associated with particulate polycyclic aromatic hydrocarbons. The compound occurs in the low temperature fraction of coal tar distillate (ref. 13).

TOXIC PROPERTIES, HEALTH EFFECTS:

Certain polycyclic aromatic hydrocarbons when administered topically to animals may induce tumors at the site of application (ref. 5). Specific activity of this compound is not reported, although the 9,10 dimethyl isomer has shown slight carcinogenic activity (ref. 5). Several dimethyl anthracenes are considered inactive (ref. 5).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

21A160
2,7-DIMETHYLANTHRACENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

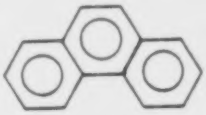
CATEGORY: 21A

WLN: LB666J

PHENANTHRENE: $C_{14}H_{10}$. 21A180

Monoclinic crystals from alcohol; solutions exhibit faint blue fluorescence.

STRUCTURE:



PROPERTIES:

Molecular wt: 178; mp: 101; bp: 340; d: 0.9800^4; vap. press.: 1 mm at 118.3; vap. d: 6.14; insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 1); lipid solubility: 2 percent solution in olive oil (ref. 14).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Phenanthrene is among the lower molecular weight polycyclic hydrocarbons comprising the volatile portion of the benzene-soluble fraction of coal tar (ref. 2). Concentrations of 0.6102 $\mu g/1{,}500\ m^3$ and 6 $\mu g/1{,}000\ m^3$ in urban air are reported (ref. 3). This is equivalent to 0.0004 to 0.006 $\mu g/m^3$. Phenanthrene is associated with particulate polycyclic aromatic hydrocarbons, PPAH, (ref. 4). The following concentrations of PPAH have been estimated or reported: Air (urban environment in winter in seven selected U.S. cities): 21.6 ng/m^3 - 146 ng/m^3 (ref. 4); groundwater and surface-treated water: 0.001 $\mu g/\ell$ - 0.025 $\mu g/\ell$ (ref. 1); upper layer of Earth's crust: 100 $\mu g/kg$ - 1,000 $\mu g/kg$ (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{50} (oral, mouse): 700 mg/kg.

Phenanthrene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 5). Phenanthrene is reported to produce tumors in mice. The EPA/NIOSH ordering number is 3121. The lowest dose to induce an oncogenic response is reported as 71 mg/kg. The adjusted ordering number is 44.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Phenanthrene appears on EPA Consent Decree List with an assigned priority of 1.

TLV (coal-tar pitch volatiles): 0.2 mg/m^3. [The specification includes naphthalene, anthracene, acridine, phenanthrene, and fluorene, collectively. The purpose of the TLV is to minimize concentrations of higher weight polycyclic hydrocarbons which are carcinogenic (ref. 2)].

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/44 = 1.59 \times 10^3\ \mu g/m^3$	Air, Ecology:
Water, Health: $15 \times 1.59 \times 10^3 = 2.39 \times 10^4\ \mu g/\ell$	Water, Ecology:
Land, Health: $0.2 \times 2.39 \times 10^4 = 4.78 \times 10^3\ \mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 700 = 75\ \mu g/m^3$

$EPC_{AH3} = 0.081 \times 700 = 57\ \mu g/m^3$

$EPC_{WH1} = 15 \times 57 = 855\ \mu g/\ell$

$EPC_{WH2} = 0.4 \times 700 = 280\ \mu g/\ell$

$EPC_{LH} = 0.2 \times 280 = 56\ \mu g/g$

$EPC_{AC2} = 10^3/(6 \times 44) = 3.8\ \mu g/m^3$

$EPC_{WC} = 15 \times 3.8 = 57\ \mu g/\ell$

$EPC_{LC} = 0.2 \times 57 = 11.4\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

X
21A180
PHENANTHRENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.6E3		3.8		0.0004 to 0.006
Water, $\mu g/l$ (ppm Wt)			2.4E4		57		
Land, $\mu g/g$ (ppm Wt)			4.8E3		11.4		

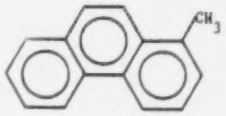
*To be multiplied by dilution factor

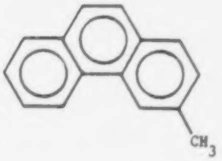
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			57		3.8
Water, $\mu g/l$ (ppm Wt)			280		57
Land, $\mu g/g$ (ppm Wt)			56		11.4

CATEGORY: 21A
METHYLPHENANTHRENES: $C_{15}H_{12}$ 21A200
1-METHYLPHENANTHRENE: A solid. 21A201
3-METHYLPHENANTHRENE: A solid. 21A202

WLN:

STRUCTURE:





PROPERTIES:

	mol.wt	mp.	bp.	solubility in water
1-methylphenanthrene	192.26	123	-	insoluble
3-methylphenanthrene	192.26	65	140-50⁶	soluble in hot water

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Methylphenanthrene has been reported in urban atmosphere at a concentration of 0.5825 μg/1,500 m^3 or 0.0004 μg/m^3 (ref. 3).

Methylphenanthrenes are likely to be associated with particulate polycyclic aromatic hydrocarbons.

TOXIC PROPERTIES, HEALTH EFFECTS:

Certain polycyclic aromatic hydrocarbons, when administered topically to animals, may induce tumors at the site of application (ref. 5).

Specific activity of 1-methyl and 3-methyl phenanthrene is not reported.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

TLV (coal-tar pitch volatiles): 0.2 mg/m^3. [The specification includes naphthalene, anthracene, acridine, phenanthrene, and fluorene, collectively. The purpose of the TLV is to minimize concentrations of higher weight polycyclic hydrocarbons which are carcinogenic (ref. 2).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

21A200
METHYLPHENANTHRENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							0.0004†
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

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† Urban atmosphere concentration. Rural background value not available.

REFERENCES: CATEGORY 21A

Fused Polycyclic Hydrocarbons - Two- and Three-Ring Fused Polycyclic Hydrocarbons

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REFERENCES: CATEGORY 21A (Continued)

12. Sax, N. I., Ed. Dangerous Properties of Industrial Materials, Fourth Edition. Van Nostrand Reinhold Co., New York, NY (1975).

13. Josephy, E., and F. Radt. Elsevier's Encyclopedia of Organic Chemisty, Vol. 13, Elsevier Publishing Co., Inc. (1940).

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17. Rodd, E. H. Chemistry of Carbon Compounds, Vol. III, Part F, Elsevier Publishing Company, Inc., New York, NY (1965).

CATEGORY 21

FUSED POLYCYCLIC HYDROCARBONS

SUBCATEGORY: 21B - Four Ring Fused Polycyclic Hydrocarbons

Summary of Subcategory

Total number of compounds in subcategory	23
number of parent compounds with subspecies	3
number of subspecies	15
Number of parent compounds with no MEG values	2
Number of parent compounds with natural background levels only	2
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	7

Consent Decree compounds included in subcategory: 3

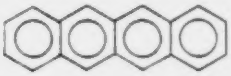
21B040	Benz(a)anthracene
21B120	Chrysene
21B180	Pyrenes

CATEGORY: 21B

WLN: L E6 C666J

NAPHTHACENE: $C_{18}H_{12}$ (2,3-benzanthracene, tetracene, chrysogen, benzo(b)anthracene).
Crystallizes from xylene in orange leaflets; solutions show slight green fluorescence. 21B020

STRUCTURE:



PROPERTIES:

Molecular wt: 228.28; mp: 341; sublimes in vacuo; insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Naphthacene occurs in coal tar.

TOXIC PROPERTIES, HEALTH EFFECTS:

Naphthacene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 2). Naphthacene is considered inactive as a carcinogen (ref. 2).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 [for particulate polycyclic aromatic hydrocarbons (PPAH). This TLV recognizes the carcinogenic potential of PPAH collectively.]

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	Air, Ecology:
Water, Health:	Water, Ecology:
Land, Health:	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

21B020
NAPHTHACENE

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

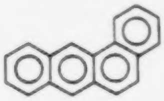
	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

CATEGORY: 21B

WLN: L D6 B666J

BENZ(a)ANTHRACENE: $C_{18}H_{12}$ (benzo(b)phenanthrene, 1,2-benzanthracene, 2,3-benzophenanthrene, BA). 21B040
Crystallizes in the form of plates from ethanol.
Solutions exhibit greenish-yellow fluorescence.

STRUCTURE:



PROPERTIES:

Molecular wt.: 228.28; mp: 158-9; bp: 400° C; sublimes; insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 1); lipid solubility: 0.6 mg/0.2 ml neutral, sterile olive oil (ref. 3).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benz(a)anthracene occurs in coal tar and is associated with particulate polycyclic aromatic hydrocarbons, PPAH. The lowest urban air concentration reported for benz(a)anthracene is 44.69 μg/1500 m^3 (ref. 4). This is equivalent to 0.029 $\mu g/m^3$.

Concentrations of BA in soils (nonindustrial areas) ranging from 5-20 μg/kg have been reported (ref. 5). BA has also been identified in river water and estuarine sediments (ref. 6).

Other concentrations of BA are reported as follows: (a) drinking water - 23.2 $\mu g/m^3$; (b) cooked meat or fish - 189 μg/kg; (c) vegetables - 230 μg/kg; (d) roasted coffee - 14.2 μg/kg (ref. 5).

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{Lo} (intravenous, mouse): 10 mg/kg.

Benz(a)anthracene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 2). Benz(a)anthracene has been shown to produce tumors in mice. The EPA/NIOSH ordering number is 3,124. The lowest dose to induce a carcinogenic response is reported as 2 mg/kg. The adjusted ordering number is 1562.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 [for particulate polycyclic aromatic hydrocarbons (PPAH). This TLV recognizes the carcinogenic potential of PPAH collectively].

Benz(a)anthracene appears on the EPA Consent Decree List with an assigned priority of 1.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/1{,}562 = 44.8\ \mu g/m^3$
Water, Health: $15 \times 44.8 = 672\ \mu g/\ell$
Land, Health: $0.2 \times 672 = 134.4\ \mu g/g$

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 10 = 1.07\ \mu g/m^3$
$EPC_{AH3} = 0.081 \times 10 = 0.81\ \mu g/m^3$
$EPC_{WH1} = 15 \times 0.81 = 12.2\ \mu g/\ell$
$EPC_{WH2} = 0.4 \times 10 = 4.0\ \mu g/\ell$
$EPC_{LH} = 0.2 \times 4 = 0.8\ \mu g/g$
$EPC_{AC2} = 10^3/(6 \times 1{,}562) = 0.11\ \mu g/m^3$
$EPC_{WC} = 15 \times 0.11 = 1.65\ \mu g/\ell$
$EPC_{LC} = 0.2 \times 1.65 = 0.33\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

XXX
21B040
BENZ(a)ANTHRACENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			4.5E1		0.11		0.029†
Water, $\mu g/l$ (ppm Wt)			6.7E2		1.65		0.023‡
Land, $\mu g/g$ (ppm Wt)			1.34E2		0.33		0.02

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			0.81		0.11
Water, $\mu g/l$ (ppm Wt)			4.0		1.65
Land, $\mu g/g$ (ppm Wt)			0.8		0.33

† Reported for urban air. No rural concentration is reported.

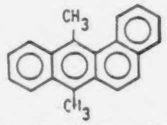
‡ Drinking water.

CATEGORY: 21B

WLN: L D6 B666J CJ

7,12-DIMETHYLBENZ(a)ANTHRACENE: $C_{20}H_{16}$, (9,10-dimethyl-1,2-benzanthracene, DMBA). 21B060
Crystallizes as greenish-yellow plates from acetone-alcohol, maximum fluorescence at 440 nm.

STRUCTURE:



PROPERTIES:

Molecular wt.: 256.33; mp: 122-123; insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 1), and by purines such as caffeine (ref. 7); lipid solubility: 50 mg/ml in tributyrin (ref. 8).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Although 7,12-dimethylbenz(a)anthracene has not been positively identified in products of coal pyrolysis, the molecular weight fraction corresponding to the compound has been isolated. It is generally presumed to be associated with particulate polycyclic aromatic hydrocarbons and with coal tar. It has been identified in soil adjacent to an oil refinery (ref. 6).

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{50} (oral,mouse): 340 mg/kg.

7,12-Dimethylbenz(a)anthracene is known to be highly carcinogenic in experimental animals (ref. 2). Experimental evidence also indicates that it is a teratogenic agent in rats (ref. 9).

The EPA/NIOSH ordering number based on carcinogenicity is 5,729. The lowest dose to induce a carcinogenic response is 21 μg/kg, and the adjusted ordering number is 272,809. The EPA/NIOSH ordering number based on teratogenicity is 4,102, with the lowest dosage being 20 mg/kg. The adjusted ordering number is 205.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/272{,}809 = 0.26\ \mu g/m^3$
Water, Health: $15 \times 0.26 = 3.9\ \mu g/\ell$
Land, Health: $0.2 \times 3.9 = 0.78\ \mu g/g$

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 340 = 36.4\ \mu g/m^3$
$EPC_{AH3} = 0.081 \times 340 = 27.5\ \mu g/m^3$
$EPC_{WH1} = 15 \times 27.5 = 413\ \mu g/\ell$
$EPC_{WH2} = 0.4 \times 340 = 136\ \mu g/\ell$
$EPC_{LH} = 0.2 \times 136 = 27.2\ \mu g/g$
$EPC_{AC2} = 10^3/(6 \times 272{,}809) = 0.0006\ \mu g/m^3$
$EPC_{WC} = 15 \times 0.006 = 0.009\ \mu g/\ell$
$EPC_{LC} = 0.2 \times 0.009 = 1.8 \times 10^{-3}\ \mu g/g$

$EPC_{AT} = 10^3/(6 \times 205) = 0.8\ \mu g/m^3$
$EPC_{WT} = 15 \times 0.8 = 12\ \mu g/\ell$
$EPC_{LT} = 0.2 \times 12 = 2.4\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

XXX
21B060
7,12-DIMETHYLBENZ(a)ANTHRACENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.6E-1		0.0006		
Water, $\mu g/l$ (ppm Wt)			3.9E0		0.009		
Land, $\mu g/g$ (ppm Wt)			7.8E-1		0.0018		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			27.5		0.0006
Water, $\mu g/l$ (ppm Wt)			136		0.009
Land, $\mu g/g$ (ppm Wt)			27.2		0.0018

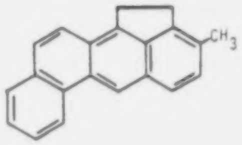
CATEGORY: 21B

WLN: L E6 D6656 1A T&&&T&J R

3-METHYLCHOLANTHRENE: $C_{21}H_{16}$ (1,2-dihydro-3-methylbenz(j)-aceanthrylene, 20-methylcholanthrene).

Straw-yellow needles from benzene. 21B080

STRUCTURE:



PROPERTIES:
Molecular wt: 268.37; mp: 176.5-177.5; d: 1.28^{20}; insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 1); lipid solubility: 12 mg/ml in tributyrin (ref. 8).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

3-Methylcholanthrene may be formed by the pyrolytic degradation of cholesterol derivatives (ref. 7). The compound may occur as a constituent of particulate polycyclic aromatic hydrocarbons, PPAH, but reports of its occurrence were not located. It is not reported to be present in natural waters or soils.

TOXIC PROPERTIES, HEALTH EFFECTS:

Systemic effects observed in mice exposed to 3-methylcholanthrene include inflammation of the liver, kidney and lungs, hyperplasia of the bone marrow, spleen, and lymph nodes (ref. 16). The disappearance rate of 3-methylcholanthrene from the site of subcutaneous injection indicates a half life of 3.5 weeks (ref. 16).

3-Methylcholanthrene is a known carcinogen. It causes chromosome aberrations in mammalian cells (ref. 10). The EPA/NIOSH ordering number is 5,829. The lowest dose to induce a response is reported as 0.312 mg/kg. The adjusted ordering number is 18,683.

Teratogenic effects in mice and in lower animals (newt, tadpoles) have also been observed (ref. 16).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/18{,}683 = 3.75\ \mu g/m^3$	Air, Ecology:
Water, Health: $15 \times 3.75 = 56\ \mu g/\ell$	Water, Ecology:
Land, Health: $0.2 \times 56 = 11.2\ \mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 18{,}683) = 0.009\ \mu g/m^3$

$EPC_{WC} = 15 \times 0.009 = 0.14\ \mu g/\ell$

$EPC_{LC} = 0.2 \times 0.14 = 0.03\ \mu g/g$

273

MULTIMEDIA ENVIRONMENTAL GOALS

XXX
21B080
3-METHYLCHOLANTHRENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			3.8E0		0.009		
Water, $\mu g/l$ (ppm Wt)			5.6E1		0.14		
Land, $\mu g/g$ (ppm Wt)			1.1E1		0.03		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					0.009
Water, $\mu g/l$ (ppm Wt)					0.14
Land, $\mu g/g$ (ppm Wt)					0.03

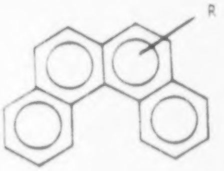
CATEGORY: 21B

BENZO(c)PHENANTHRENE AND ALKYL DERIVATIVES: Solids. 21B100

BENZO(c)PHENANTHRENE:	$C_{18}H_{12}$.	21B101
1-METHYL-BENZO(c)PHENANTHRENE	$C_{19}H_{14}$.	21B102
2-METHYL-BENZO(c)PHENANTHRENE	$C_{19}H_{14}$.	21B103
5-METHYL-BENZO(c)PHENANTHRENE	$C_{19}H_{14}$.	21B104
6-METHYL-BENZO(c)PHENANTHRENE	$C_{19}H_{14}$.	21B105
7-METHYL-BENZO(c)PHENANTHRENE	$C_{19}H_{14}$.	21B106
8-METHYL-BENZO(c)PHENANTHRENE	$C_{19}H_{14}$.	21B107
2-ETHYL-BENZO(c)PHENANTHRENE	$C_{20}H_{17}$.	21B108
6-ETHYL-BENZO(c)PHENANTHRENE	$C_{20}H_{17}$.	21B109
n-PROPYL-BENZO(c)PHENANTHRENE	$C_{21}H_{18}$.	21B10a
ISOPROPYL-BENZO(c)PHENANTHRENE	$C_{21}H_{18}$.	21B10b

WLN: L C6 B666J

STRUCTURE:



where R is alkyl group.

PROPERTIES:

Compound	Molecular wt.	mp
benzo(c)phenanthrene	228.30	68
1-methyl-benzo(c)phenanthrene	242.33	77-78
2-methyl-benzo(c)phenanthrene	242.33	71
5-methyl-benzo(c)phenanthrene	242.33	140-141
6-methyl-benzo(c)phenanthrene	242.33	81-82
7-methyl-benzo(c)phenanthrene	242.33	54
8-methyl-benzo(c)phenanthrene	242.33	107-108
2-ethyl-benzo(c)phenanthrene	257.37	67-68
6-ethyl-benzo(c)phenanthrene	257.37	82-83
n-propyl-benzo(c)phenanthrene	270.39	67-68
isopropyl-benzo(c)phenanthrene	270.39	76-77

All insoluble in water although solubility may be enhanced by surfactant impurities in water (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

The urban air concentration of benzo(c)phenanthrene is reported as 9.781 µg/1,500 m³ (ref. 4). This is equivalent to 6.5 ng/m³. Benzo(c)phenanthrene and its alkyl derivatives probably occur as constituents of particulate polycyclic aromatic hydrocarbons, PPAH.

X-ray analysis shows that benzo(c)phenanthrene is not planar. The four rings are inclined to each other. The compound therefore has a dipole moment.

TOXIC PROPERTIES, HEALTH EFFECTS:

Benzo(c)phenanthrene is rated by the National Academy of Science as strongly carcinogenic (ref. 11). (Presumably, alkyl derivatives as well as the parent compound are treated collectively in the rating.) Benzo(c)phenanthrene and eight of its alkyl derivatives have produced tumors in mice (ref. 12). The EPA/NIOSH ordering number is 3,119; the lowest dosage to induce an oncogenic response is 10 mg/kg (for 5-methyl benzo(c)phenanthrene). The adjusted ordering number for the compounds collectively is 312.

Oncogenic properties of benzo(c)phenanthrene are increased by the introduction of alky groups.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m³ (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$7 \times 10^4/312 = 224\ \mu g/m^3$	Air, Ecology:
Water, Health:	$15 \times 224 = 3{,}360\ \mu g/l$	Water, Ecology:
Land, Health:	$0.2 \times 3{,}360 = 672\ \mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 312) = 0.5\ \mu g/m^3$

$EPC_{WC} = 15 \times 0.5 = 7.5\ \mu g/l$

$EPC_{LC} = 0.2 \times 7.5 = 1.5\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

X

21B100

BENZO(c)PHENANTHRENE & ALKYL DERIVATIVES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.24E2		0.5		0.006
Water, $\mu g/l$ (ppm Wt)			3.36E3		7.5		
Land, $\mu g/g$ (ppm Wt)			6.73E2		1.5		

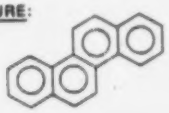
*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					0.5
Water, $\mu g/l$ (ppm Wt)					7.5
Land, $\mu g/g$ (ppm Wt)					1.5

CATEGORY: 21B

WLN: L E6 B666J

STRUCTURE:



CHRYSENE: $C_{18}H_{12}$ (1,2-benzophenanthrene, benz(a) phenanthrene). 21B120
Crystallizes in the form of plates; solutions and crystals exhibit blue fluorescence.

PROPERTIES:

Molecular wt: 228.28; mp: 255-256; sublimes in vacuo; bp: 448; d: 1.274^{20}; insoluble in water, solubility may be enhanced by surfactant impurities in water (ref. 1); lipid solubility: 7.5 percent solution in olive oil (ref. 5).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Chrysene occurs in coal tar, is formed during distillation of coal, and is a product of pyrolysis of many fats and oils. Chrysene is associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 13).

Environmental concentrations of chrysene are reported as follows: urban air--0.23 ng/m^3 (ref. 4). surface water--11.8-38.2 μg/m^3; sand--15 μg/kg (ref. 5).

Maximum concentrations of chrysene in foods are also reported: cooked meat or fish--173 μg/kg; vegetables--395 μg/kg; roasted coffee--19.1 μg/kg (ref. 5).

Chrysene has also been identified in the mineral Curtisite (ref. 6).

TOXIC PROPERTIES, HEALTH EFFECTS:

Chrysene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 2). Chrysene is reported to produce tumors in mice. The EPA/NIOSH ordering number is 3,122. The lowest dose to induce an oncogenic response is reported as 99 mg/kg. The adjusted ordering number is 31.5.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Chrysene appears on the EPA Consent Decree List with an assigned priority of 1.

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/31.5 = 2.22 \times 10^3$ μg/m^3	Air, Ecology:
Water, Health: $15 \times 2.22 \times 10^3 = 3.33 \times 10^4$ μg/ℓ	Water, Ecology:
Land, Health: $0.2 \times 3.33 \times 10^4 = 6.66 \times 10^3$ μg/g	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 31.5) = 5.29$ μg/m^3
$EPC_{WC} = 15 \times 5.29 = 79.4$ μg/ℓ
$EPC_{LC} = 0.2 \times 79.4 = 15.88$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

21B120
CHRYSENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.22E3		5.29		$2.3x10^{-4}$†
Water, $\mu g/l$ (ppm Wt)			3.33E4		79.4		0.01 to 0.04
Land, $\mu g/g$ (ppm Wt)			6.6E3		15.88		0.015

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					5.29
Water, $\mu g/l$ (ppm Wt)					79.4
Land, $\mu g/g$ (ppm Wt)					15.88

† Reported for urban air. No rural concentration is reported.

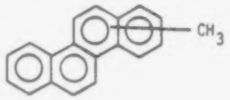
CATEGORY: 21B

METHYL CHRYSENES: $C_{19}H_{14}$ (methyl-1,2-benzophenanthrene). 21B140

The 4-methyl and 5-methyl chrysenes exhibit fluorescence.
4-METHYL CHRYSENE. 21B141
5-METHYL CHRYSENE. 21B142

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 242; mp: 117-254; insoluble in water;
solubility may be enhanced by surfactant impurities in water (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Methyl chrysenes are associated with particulate polycyclic aromatic hydrocarbons and with coal tar. The urban-air concentration for methyl chrysenes is reported as 6.195 μg/1500 m^3 (ref. 4). This is equivalent to 4.1 ng/m^3. Methyl chrysenes have also been detected in the polycyclic aromatic hydrocarbon fraction of marine sediments (ref. 14).

TOXIC PROPERTIES, HEALTH EFFECTS:

Methyl chrysenes may be present in soot, coal tar, oils, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 2). Five methyl chrysenes are reported to cause tumors in mice. The collective EPA/NIOSH ordering number for the five compounds is 3123. The lowest dose to induce an oncogenic response is reported as 80 mg/kg. The adjusted ordering number for the methyl chrysenes collectively is 39.

Carcinogenic activity may be increased or decreased depending on the methylation site. In tests involving chrysene and six methyl isomers, 5-methyl chrysene was shown to be the most potent carcinogen (ref. 17).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$7 \times 10^4/39 = 1.79 \times 10^3$ μg/m^3	Air, Ecology:	
Water, Health:	$15 \times 1.79 \times 10^3 = 2.69 \times 10^4$ μg/ℓ	Water, Ecology:	
Land, Health:	$0.2 \times 2.69 \times 10^4 = 5.4 \times 10^3$ μg/g	Land, Ecology:	

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 39) = 4.3$ μg/m^3
$EPC_{WC} = 15 \times 4.3 = 64.5$ μg/ℓ
$EPC_{LC} = 0.2 \times 64.5 = 12.9$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

21B140
METHYL CHRYSENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.8E3		4.3		0.004 †
Water, $\mu g/l$ (ppm Wt)			2.7E4		64.5		
Land, $\mu g/g$ (ppm Wt)			5.4E3		12.9		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					4.3
Water, $\mu g/l$ (ppm Wt)					64.5
Land, $\mu g/g$ (ppm Wt)					12.9

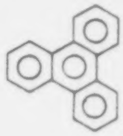
† Reported for urban atmosphere. No rural concentration is reported.

CATEGORY: 21B

WLN: L B6 H666J

TRIPHENYLENE: $C_{18}H_{12}$ (1,2:3,4-dibenznaphthalene; 9,10-benzophenanathrene). 218160
Crystallizes in the form of long needles; solutions exhibit blue fluoresence.

STRUCTURE:



PROPERTIES:

Molecular wt: 228.28; mp: 199; sublimes; bp: 425; d: 1.302; insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Triphenylene occurs to a small extent in coal tar. It has been identified in urban air in concentrations of 0.24 μg/100 m^3 (ref. 6.). This is equivalent to 0.0024 μg/m^3.

TOXIC PROPERTIES, HEALTH EFFECTS:

Triphenylene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 2).

Triphenylene is considered inactive as a carcinogen (ref. 2).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 [for particulate polycyclic aromatic hydrocarbons (PPAH). This TLV recognizes the carcinogenic potential of PPAH collectively.]

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	Air, Ecology:
Water, Health:	Water, Ecology:
Land, Health:	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

21B160
TRIPHENYLENE

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)							0.0024†
Water, μg/l (ppm Wt)							
Land, μg/g (ppm Wt)							

*To be multiplied by dilution factor

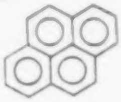
	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)					
Water, μg/l (ppm Wt)					
Land, μg/g (ppm Wt)					

†Reported for urban air.

CATEGORY: 21B

WLN: L666 B6 2AB PJ

STRUCTURE:



PYRENE: $C_{16}H_{10}$ (benzo(def)phenanthrene). 21B180

Crystallizes as pale yellow plates; solutions show slight blue fluorescence.

PROPERTIES:

Molecular wt: 202; mp: 149-50; sublimes; bp: > 360; d: 1.271^{23}_{4}; insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Pyrene occurs in coal tar. It is also obtained by the destructive hydrogenation of hard coal. The lowest reported concentration of pyrene in urban areas is 0.45 mg/m^3 (ref. 4). This is equivalent to 450 μg/m^3.

Pyrene is associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 13). The following concentrations of carcinogenic PPAH have been estimated or reported: air (urban environment in winter in seven selected U.S. cities): 21.6 ng/m^3 - 146 ng/m^3 (ref. 13); ground-water and surface-treated water: 0.001 μg/ℓ - 0.025 μg/ℓ (ref. 1); upper layer of earth's crust: 100 μg/kg - 1,000 μg/kg (ref. 1). It has also been identified in marine and estuarine sediments, in industrial associated soils, and in snow (ref. 6).

TOXIC PROPERTIES, HEALTH EFFECTS:

Pyrene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 2). Although not considered a highly active carcinogen, in high dosages it has produced tumors in mice. The EPA/NIOSH ordering number is 3,121. The lowest toxic dose reported to produce an oncogenic response is 10 g/kg. This is equivalent to 10,000 mg. The adjusted ordering number is 0.3.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Pyrene appears on the EPA Consent Decree List with an assigned priority of 1.

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/0.3 = 2.3 \times 10^5$ μg/m^3

Water, Health: $15 \times 2.3 \times 10^5 = 3.45 \times 10^6$ μg/ℓ

Land, Health: $0.2 \times 3.45 \times 10^6 = 6.9 \times 10^5$ μg/g

Air, Ecology:

Water, Ecology:

Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 0.3) = 555.6$ μg/m^3

$EPC_{WC} = 15 \times 555.6 = 8,333$ μg/ℓ

$EPC_{LC} = 0.2 \times 833 = 167$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

21B180
PYRENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			2.3E5		556		450 †
Water, μg/l (ppm Wt)			3.45E6		8,333		
Land, μg/g (ppm Wt)			6.9E5		167		

*To be multiplied by dilution factor

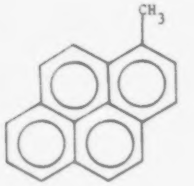
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. *Zero Threshold Pollutants* Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)					556
Water, μg/l (ppm Wt)					8,333
Land, μg/g (ppm Wt)					167

† Value reported for urban atmosphere. Rural atmosphere concentration not reported.

CATEGORY: 21B
1-METHYLPYRENE: $C_{17}H_{12}$ 21B200
Solid crystals.

WLN:

STRUCTURE:



PROPERTIES:
Molecular wt: 216.096; mp: 71-72; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Methylpyrene has been reported in urban atmosphere at a concentration of 2.622 μg/1,500 m^3 (ref. 4). This is equivalent to 0.0017 μg/m^3.
Methylpyrene is likely to be associated with particulate polycyclic aromatic hydrocarbons.

TOXIC PROPERTIES, HEALTH EFFECTS:

Certain polycyclic aromatic hydrocarbons when administered topically to animals may induce tumors at the site of application (ref. 2). Evidence of carcinogenic potential for 1-methylpyrene is not available. 2-Methylpyrene is considered inactive (ref. 2).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

21B200
1-METHYLPYRENE

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							0.0017†
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

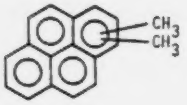
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

†Reported for urban air.

CATEGORY: 21B

WLN:

STRUCTURE:



DIMETHYL PYRENES: $C_{18}H_{14}$. 21B220
Crystallize in the form of plates from petroleum ether.
3,4-DIMETHYL PYRENE : 21B221
4,5-DIMETHYL PYRENE : 21B222

PROPERTIES:

Molecular wt: 232; insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Alkyl pyrenes have been isolated from coal tar and from soot (ref. 15).

Dimethyl pyrenes are associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 13). The following concentrations of carcinogenic PPAH have been estimated or reported: Air (urban environment in winter in seven selected U.S. cities): 21.6 ng/m^3 - 146 ng/m^3 (ref. 13); ground-water and surface-treated water: 0.001 µg/ℓ - 0.025 µg/ℓ (ref. 1): upper layer of Earth's crust: 100 µg/kg - 1,000 µg/kg (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

Dimethyl pyrenes may be present in soot, coal tar, and pitch which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 2). There is no evidence to indicate that the dimethylpyrenes alone are carcinogenic.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 [for particulate polycyclic aromatic hydrocarbons (PPAH). This TLV recognizes the carcinogenic potential of PPAH collectively].

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	Air, Ecology:
Water, Health:	Water, Ecology:
Land, Health:	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

21B220
DIMETHYL PYRENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

REFERENCES: CATEGORY 21B

Fused Polycyclic Hydrocarbons - Four Ring Fused Polycyclic Hydrocarbons

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CATEGORY 21

FUSED POLYCYCLIC HYDROCARBONS

SUBCATEGORY: 21C - Five Ring Fused Polycyclic Hydrocarbons

Summary of Subcategory

Total number of compounds in subcategory	8
number of parent compounds with subspecies	0
number of subspecies	0
Number of parent compounds with no MEG values	1
Number of parent compounds with natural background levels only	1
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	6

Consent Decree compounds included in subcategory: 2

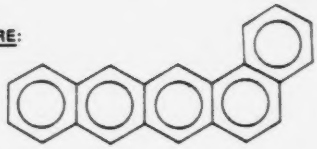
21C080	Dibenz(a,h)anthracene
21C100	Benzo(a)pyrene

CATEGORY: 21C

1,2-BENZONAPHTHACENE: $C_{22}H_{14}$ 21C020
(2,3-naptho-2,3-phenanthrene; naphtho-1',2':2,3-anthracene; 1.2:6,7-dibenzanthracene; dibenz(a,j)anthracene).
A yellow solid.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 278.35; mp: 263-4; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

1,2-Benzonaphthacene is likely to be associated with particulate polycyclic aromatic hydrocarbons. The compound has been found in the pyrene and picene fractions of coal-tar distillate (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

1,2-Benzonaphthacene has been reported to be noncarcinogenic in experimental animals (ref. 2).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

21C020
1,2-BENZONAPHTHACENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

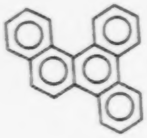
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

CATEGORY: 21C

WLN: L C6 I6 B666j

BENZO(g)CHRYSENE: $C_{22}H_{14}$ (1,2:3,4-dibenzophenanthrene). 21C040
Crystallizes as colorless needles from glacial acetic acid.

STRUCTURE:



PROPERTIES:

Molecular wt: 278.36; mp: 114.5; bp: 135; insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 3).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzo(g)chrysene probably occurs as a constituent of particulate polycyclic aromatic hydrocarbons, PPAH.

TOXIC PROPERTIES, HEALTH EFFECTS:

Although not considered to be a highly active carcinogen alone, benzo(g)chrysene is is reported to cause tumors in mice. The EPA/NIOSH ordering number is 3123. The lowest dose to induce a carcinogenic response is reported as 720 mg/kg (ref. 14). The adjusted ordering number is 4.34.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 [for particulate polycyclic aromatic hydrocarbons (PPAH). This TLV recognizes the carcinogenic potential of PPAH collectively.]

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/4.34 = 1.6 \times 10^4$ μg/m^3
Water, Health: $15 \times 1.6 \times 10^4 = 2.42 \times 10^5$ μg/ℓ
Land, Health: $0.2 \times 2.42 \times 10^5 = 4.84 \times 10^4$ μg/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 4.34) = 38.4$ μg/m^3
$EPC_{WC} = 15 \times 38.4 = 576$ μg/ℓ
$EPC_{LC} = 0.2 \times 576 = 115.2$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

21C040
BENZO(g)CHRYSENE

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.6E4		38		
Water, $\mu g/l$ (ppm Wt)			2.4E5		576		
Land, $\mu g/g$ (ppm Wt)			4.8E4		115		

*To be multiplied by dilution factor

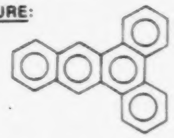
AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					38
Water, $\mu g/l$ (ppm Wt)					576
Land, $\mu g/g$ (ppm Wt)					115

CATEGORY: 21C

WLN: L D6 J6 C666J

STRUCTURE:



DIBENZ(a,c)ANTHRACENE: $C_{22}H_{14}$ (1,2:3,4-dibenzanthracene, benzo(b)triphenylene). 21C060

Crystallizes as colorless needles from ethanol; solutions show blue fluorescence.

PROPERTIES:

Molecular wt: 278.36; mp: 200-2; insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 3); lipid solubility: 0.6 mg in 0.2 ml olive oil (ref. 4).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Dibenz(a,c)anthracene is associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 5). The following concentrations of PPAH have been estimated or reported: air (urban environment in winter in seven selected U.S. cities): 21.6 ng/m^3 - 146 ng/m^3 (ref. 5); ground-water and surface-treated water: 0.001 $\mu g/\ell$ - 0.025 $\mu g/\ell$ (ref. 3); upper layer of earth's crust: 100 $\mu g/kg$ - 1,000 $\mu g/kg$ (ref. 3).

The concentration of dibenz(a,c)anthracene in urban air is reported as 13,348 $\mu g/1{,}500\ m^3$ (ref. 6). This is equivalent to 0.88 ng/m^3.

TOXIC PROPERTIES, HEALTH EFFECTS:

Dibenz(a,c)anthracene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 7).

Dibenz(a,c)anthracene is reported to cause tumors in mice. The EPA/NIOSH ordering number is 3121. The lowest dose to induce a carcinogenic response is 440 mg/kg (ref. 14). The adjusted ordering number is 7.09. There is disagreement regarding the carcinogenicity of dibenz(a,c)anthracene (ref. 7).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/7.09 = 9.9 \times 10^3\ \mu g/m^3$	Air, Ecology:
Water, Health: $15 \times 9.9 \times 10^3 = 1.5 \times 10^5\ \mu g/\ell$	Water, Ecology:
Land, Health: $0.2 \times 1.5 \times 10^5 = 3.0 \times 10^4\ \mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 7.09) = 23.5\ \mu g/m^3$

$EPC_{WC} = 15 \times 23.5 = 353\ \mu g/\ell$

$EPC_{LC} = 0.2 \times 353 = 70.6\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

21C060
DIBENZ(a,c)ANTHRACENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			9.9E3		23.5		0.009†
Water, $\mu g/l$ (ppm Wt)			1.5E5		353		
Land, $\mu g/g$ (ppm Wt)			3.0E4		71		

*To be multiplied by dilution factor

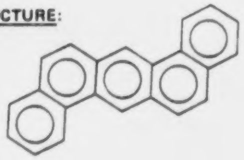
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					23.5
Water, $\mu g/l$ (ppm Wt)					353
Land, $\mu g/g$ (ppm Wt)					71

† Reported For Urban Atmosphere. No Rural Concentration Is Reported.

CATEGORY: 21C

WLN:

STRUCTURE:



DIBENZ(a,h)ANTHRACENE: $C_{22}H_{14}$ (1,2:5,6-dibenzanthracene, DB(a,h)A). 21C080

Crystallizes in the form of silvery leaflets from acetic acid.

PROPERTIES:

Molecular wt: 278.36; mp: 262; sublimes; solubility in water: 0.0005 mg/ℓ at 27° (ref. 8); lipid solubility: 8 mg/ml in tributyrin (ref. 9).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Environmental concentration of DB(a,h)A are reported as follows: urban air--3.2-32 μg/1,000 m^3; soils (Iceland)--0-2.3 μg/kg (ref. 8). DB(a,h)A has also been detected in cooked meats and vegetables (ref. 8).

The compound is probably a constituent of particulate polycyclic aromatic hydrocarbons, PPAH.

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{Lo} (intravenous, mouse): 10 mg/kg.

Dibenz(a,h)anthracene may be present in soot, coal tar, and pitch which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 7). DB(a,h)A is considered an active carcinogen and causes aberrations in mammalian cells (ref. 10). The EPA/NIOSH ordering number is 4529. The lowest dose to induce an oncogenic response is reported as 0.006 mg/kg (ref. 14). The adjusted ordering number is 754,833.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Dibenz(a,h)anthracene appears on EPA Consent Decree List with an assigned priority of 1.

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 7 x 10^4/754,833 = 0.093 μg/m^3

Water, Health: 15 x 0.093 = 1.4 μg/ℓ

Land, Health: 0.2 x 1.4 = 0.28 μg/g

Air, Ecology:

Water, Ecology:

Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

EPC_{AH2} = 0.107 x 10 = 1.07 μg/m^3

EPC_{AH3} = 0.081 x 10 = 0.81 μg/m^3

EPC_{WH1} = 15 x 0.81 = 12.2 μg/ℓ

EPC_{WH2} = 0.4 x 10 = 4.0 μg/ℓ

EPC_{LH} = 0.2 x 4.0 = 0.8 μg/g

EPC_{AC2} = 10^3/(6 x 754,833) = 0.0002 μg/m^3

EPC_{WC} = 15 x 0.0002 = 0.003 μg/ℓ

EPC_{LC} = 0.2 x 0.003 = 6 x 10^{-4} μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

XXX
21C080
DIBENZ(a,h)ANTHRACENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			9.3E-2		0.0002		0.0032 to 0.032 †
Water, $\mu g/l$ (ppm Wt)			1.4E0		0.003		0 to 0.0023
Land, $\mu g/g$ (ppm Wt)			2.8E-1		$6x10^{-4}$		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			0.8		0.0002
Water, $\mu g/l$ (ppm Wt)			4		0.003
Land, $\mu g/g$ (ppm Wt)			0.8		$6x10^{-4}$

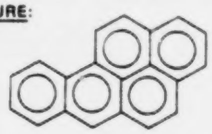
† Reported For Urban Atmosphere. No Rural Concentration Is Reported.

CATEGORY: 21C

WLN: L D6 B6666 2AB -TJ

BENZO(a)PYRENE: $C_{20}H_{12}$ (1,2-benzpyrene; B(a)P; 3,4-benzpyrene). 21C100
Yellowish plates; benzene solutions exhibit violet fluorescence.

STRUCTURE:



PROPERTIES:

Molecular wt: 252.30; mp: 179; bp: 496-510; vap. press: 10 mm at 310-312°C; insoluble in water, solubility may be enhanced by surfactant impurities in water (ref. 3); lipid solubility: 25 mg/ml in tributyrin (ref. 9).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzo(a)pyrene occurs in coal tar and in all kinds of soot and smoke. Environmental concentration of B(a)P is reported as follows: urban air--0.04-0.4 μg/1,000 m^3 (refs.6,11); forest, woods, sand (nonindustrial areas)--0-127 μg/kg (ref. 8). Other maximum concentrations reported include: drinking water--23.4 μg/m^3; cooked meat or fish--107 μg/kg; vegetables--8 μg/kg; roasted coffee--15 μg/kg (ref. 8).

The chemical half-life of benzo(a)pyrene in the atmosphere is reported as less than 1 day with solar radiation and several days without solar radiation (ref. 2). Benzo(a)pyrene is associated with particulate polycyclic aromatic hydrocarbons, PPAH. It has been identified in estuarine and marine sediments, in agricultural and industrial soil, geologic deposits, and in asbestos (ref. 13).

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{50} (subcutaneous, rat): 50 mg/kg.

Benzo(a)pyrene is considered to be an active carcinogen. It has been shown to cause chromosome aberrations in mammalian cells (ref. 10). Experimental evidence indicates that B(a)P is a mutagenic and teratogenic agent in the mouse (ref. 14). The EPA/NIOSH ordering number based on carcinogenic responses is 6629. The lowest dose to induce a carcinogenic response is reported as 2 μg/kg (ref. 14). The adjusted ordering number is 3,314,500 based on carcinogenicity. The EPA/NIOSH ordering number based on teratogenicity is 3102. The lowest dose resulting in teratogenic effects is 240 mg/kg (ref. 14). The adjusted ordering number based on teratogenicity is 12.9.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Benzo(a)pyrene appears on EPA Consent Decree List with an assigned priority of 1.

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/3{,}314{,}500 = 0.02$ μg/m^3
Water, Health: $15 \times 0.02 = 0.3$ μg/ℓ
Land, Health: $0.2 \times 0.3 = 0.06$ μg/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 50 = 5.35$ μg/m^3
$EPC_{AH3} = 0.081 \times 50 = 4.1$ μg/m^3
$EPC_{WH1} = 15 \times 4.1 = 61.5$ μg/ℓ
$EPC_{WH2} = 0.4 \times 50 = 20$ μg/ℓ
$EPC_{LH} = 0.2 \times 20 = 4.0$ μg/g
$EPC_{AC2} = 10^3/(6 \times 3{,}314{,}500) = 5 \times 10^{-5}$ μg/m^3
$EPC_{WC} = 15 \times 5 \times 10^{-5} = 7.5 \times 10^{-4}$ μg/ℓ
$EPC_{LC} = 0.2 \times 7.5 \times 10^{-4} = 1.5 \times 10^{-4}$ μg/g

$EPC_{AT} = 10^3/(6 \times 12.9) = 12.9$ μg/m^3
$EPC_{WT} = 15 \times 12.9 = 194$ μg/ℓ
$EPC_{LT} = 0.2 \times 194 = 38.3$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

XXX
21C100
BENZO(a)PYRENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.0E-2		5.0×10^{-5}		4×10^{-5} to 4×10^{-4}†
Water, $\mu g/l$ (ppm Wt)			3.0E-1		7.5×10^{-4}		0.02‡
Land, $\mu g/g$ (ppm Wt)			6.0E-2		1.5×10^{-4}		0 to 0.13§

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			4.1		5.0×10^{-5}
Water, $\mu g/l$ (ppm Wt)			20		7.5×10^{-4}
Land, $\mu g/g$ (ppm Wt)			4		1.5×10^{-4}

† Reported For Urban Atmosphere

‡ Drinking Water

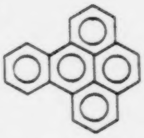
§ Sand, non-industrial Areas

CATEGORY: 21C

WLN:

BENZO(e)PYRENE: $C_{20}H_{12}$ (4,5-benzopyrene; 1,2-benzpyrene). 21C120
Prisms or plates from benzene.

STRUCTURE:



PROPERTIES:

Molecular wt: 252.32; mp: 178-9; sublimes at 250° (4 mm); insoluble in water, solubility may be enhanced by surfactant impurities in water (ref. 3); lipid solubility: 2.5 percent in olive oil (ref. 15).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzo(e)pyrene is a constituent of the high-boiling coal tar (ref. 16). It has been isolated from soils (ref. 17). The lowest reported urban concentration for benzo(e)pyrene is 0.90 ng/m^3 (ref. 6).

Benzo(e)pyrene is associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 5). The following concentrations of carcinogenic PPAH have been estimated or reported: Air (urban environment in winter in seven selected U.S. cities): 21.6 ng/m^3 - 146 ng/m^3 (ref. 5); ground-water and surface-treated water: 0.001 μg/ℓ - 0.025 μg/ℓ (ref. 3): upper layer of earth's crust: 100 μg/kg - 1,000 μg/kg (ref. 3).

TOXIC PROPERTIES, HEALTH EFFECTS:

Benzo(e)pyrene may be present in soot, coal tar, and pitch which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 7).

Benzo(e)pyrene is reported to cause tumors in mice and guinea pigs. The EPA/NIOSH ordering number is 3223. The lowest dose to induce an oncogenic response is reported as 140 mg/kg (ref. 14). The adjusted ordering number is 23.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/23 = 3.04 \times 10^3$ μg/m^3	Air, Ecology:
Water, Health: $15 \times 3.04 \times 10^3 = 4.56 \times 10^4$ μg/ℓ	Water, Ecology:
Land, Health: $0.2 \times 4.57 \times 10^4 = 9.14 \times 10^3$ μg/g	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 23) = 7.25$ μg/m^3
$EPC_{WC} = 15 \times 7.25 = 109$ μg/ℓ
$EPC_{LC} = 0.2 \times 109 = 21.8$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

21C120
BENZO(e)PYRENE

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			3.0E3		7		9.0×10^{-4}
Water, $\mu g/l$ (ppm Wt)			4.6E4		109		
Land, $\mu g/g$ (ppm Wt)			9.1E3		22		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					7
Water, $\mu g/l$ (ppm Wt)					109
Land, $\mu g/g$ (ppm Wt)					22

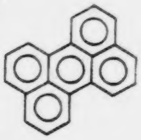
303<

CATEGORY: 21C

WLN: L666 L6 K6 2AL

PERYLENE: $C_{20}H_{12}$ (peri-dinaphthalene, dibenz(de,kl) anthracene). Yellow to colorless plates from toluene. 21C140

STRUCTURE:



PROPERTIES:

Molecular wt: 252.34; mp: 277-279; sublimes 350-400° C; d: 1.35; insoluble in water, solubility may be enhanced by surfactant impurities in water (ref. 3).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Perylene occurs in coal tar and in high-boiling petroleum fractions. The lowest reported urban level for perylene is given as 0.10 ng/m^3 (ref. 6).

Perylene is associated with particulate polycyclic aromatic hydrocarbons PPAH (ref. 5). The following concentrations of carcinogenic PPAH have been estimated or reported: Air (urban environment in winter in seven selected U.S. cities): 21.6 ng/m^3 - 146 ng/m^3 (ref. 5); ground-water and surface-treated water: 0.001 μg/ℓ - 0.025 μg/ℓ (ref. 3): upper layer of earth's crust: 100 μg/kg - 1000 μg/kg (ref. 3).

TOXIC PROPERTIES, HEALTH EFFECTS:

There is no report of oncogenic responses in animals or humans which are attributable to this compound.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:
Water, Health:
Land, Health:

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

21C140
PERYLENE

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)							0.0001 †
Water, μg/l (ppm Wt)							
Land, μg/g (ppm Wt)							

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)					
Water, μg/l (ppm Wt)					
Land, μg/g (ppm Wt)					

† Reported For Urban Atmosphere. No Rural Concentration Is Reported.

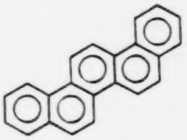
CATEGORY: 21C

WLN: L F6 E6 B666J

PICENE: $C_{22}H_{14}$ (1,2:7,8-dibenzphenanthrene, dibenzo(a,i) phenanthrene). 21C160

Crystallizes in the form of plates with bluish fluorescence.

STRUCTURE:



PROPERTIES:

Molecular wt: 278.33; mp: 367; sublimes 300° C; bp: 518-20; insoluble in water, solubility may be enhanced by surfactant impurities in water (ref. 3).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Picene is found in tar oils from soft coal and in petroleum.
The rural concentration for picene is reported as 0.0974 $\mu g/1{,}500\ m^3$ (ref. 6). This is equivalent to 0.06 ng/m^3. Picene probably occurs as a constituent of particulate polycyclic aromatic hydrocarbons. It has been identified in urban air and in the mineral curtisite (ref. 13).

TOXIC PROPERTIES, HEALTH EFFECTS:

Picene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 7).

Picene is reported to cause tumors in mice. The EPA/NIOSH ordering number is 3121. The lowest dose to induce an oncogenic response is reported as 111 mg/kg (ref. 14). The adjusted ordering number is 28.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/28 = 2.5 \times 10^3\ \mu g/m^3$
Water, Health: $15 \times 2.5 \times 10^3 = 3.75 \times 10^4\ \mu g/\ell$
Land, Health: $0.2 \times 3.75 \times 10^4 = 7.5 \times 10^3\ \mu g/g$

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 28) = 5.95\ \mu g/m^3$
$EPC_{WC} = 15 \times 5.95 = 89.3\ \mu g/\ell$
$EPC_{LC} = 0.2 \times 89.3 = 17.9\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

21C160
PICENE

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.5E3		6		6.5×10^{-5}
Water, $\mu g/l$ (ppm Wt)			3.75E4		89		
Land, $\mu g/g$ (ppm Wt)			7.5E3		18		

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					6
Water, $\mu g/l$ (ppm Wt)					89
Land, $\mu g/g$ (ppm Wt)					18

REFERENCES: CATEGORY 21C

Fused Polycyclic Hydrocarbons - Five Ring Fused Polycyclic Hydrocarbons

1. Clar, E. Chemische Berichte, 62: 1574 (1929).

2. Cook, C. Proceedings of the Royal Society, London. III, 455 (1932).

3. Andelman, J. B., and M. J. Suess. Polynuclear Aromatic Hydrocarbons in the Water Environment. Bull Wld. Hlth. Org. 43: 479-508 (1970).

4. National Cancer Institute. Survey of Compounds Which Have Been Tested for Carcinogenic Activity: 1970-1971 Volume. Prepared by Tracor Jitco Inc., Rockville, MD under Contract No. NIH-NCI-E-71-2266 for National Cancer Institute. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC. Public Health Service Publication No. 149.

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6. Wagoner, D. Compilation of Ambient Trace Substances. Draft of Report Prepared by Research Triangle Institute Under Contract No. 68-02-1325 for U.S. Environmental Protection Agency. Available from W. G. Tucker, Project Officer, IERL-EPA, Research Triangle Park, N.C. (1976).

7. Searle, C. E., Ed. Chemical Carcinogens. ACS Monograph 173. American Chemical Society, Washington, DC (1976).

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REFERENCES: CATEGORY 21C (Continued)

13. Kingsbury, G. L., R. C. Sims, and J. B. White. Source and Ambient Concentration Data for Polycyclic Organic Matter. Vol. I-III. Draft of Report Prepared by Research Triangle Institute, under Contract No. 68-02-2612 for U.S. Environmental Protection Agency. Available from J. O. Milliken, Project Officer, IERL-EPA, Research Triangle Park, N.C. (1978).

14. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

15. National Cancer Institute. Survey of Compounds Which Have Been Tested for Carcinogenic Activity: 1961-1962 Volume. Prepared by John I. Thompson and Co., Rockville, MD under Contract No. NIH-69-2086 for National Cancer Institute. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC. Public Health Service Publication No. 149.

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CATEGORY 21

FUSED POLYCYCLIC HYDROCARBONS

SUBCATEGORY: 21D - Compounds with More than Five Fused Rings

Summary of Subcategory

Total number of compounds in subcategory	5
number of parent compounds with subspecies	0
number of subspecies	0
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	2
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	3

Consent Decree compounds included in subcategory: 1

21D080 Benzo(ghi)perylene

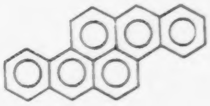
CATEGORY: 21D

WLN: L D6 B66 D666 2AB A&J

DIBENZO(a,h)PYRENE: $C_{24}H_{14}$, (dibenzo(b,def)chrysene; 1,2:6,7-dibenzpyrene; 3,4:8,9-dibenzpyrene; DB(a,h)P). 21D020

Crystallizes as gold-orange plates from trichlorobenzene.

STRUCTURE:



PROPERTIES:

Molecular wt: 302.37; mp: 315; insoluble in water, solubility may be enhanced by surfactant impurities in water (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Dibenzo(a,h)pyrene is a constituent of coal-tar pitch. It may be formed by pyrolysis of anthracene. Dibenzo(a,h)pyrene is associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 2). The following concentrations of carcinogenic PPAH have been estimated or reported: Air (urban environment in winter in seven selected U.S. cities): 21.6 ng/m^3 - 146 ng/m^3 (ref. 2); ground-water and surface-treated water: 0.001 μg/ℓ - 0.025 μg/ℓ (ref. 1); upper layer of Earth's crust: 100 μg/kg - 1,000 μg/kg (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

Dibenzo(a,h)pyrene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 3).

Dibenzo(a,h)pyrene is reported to cause tumors in mice. The EPA/NIOSH ordering number is 3121. The lowest dose to induce a carcinogenic response is reported as 165 mg/kg (ref. 9). The adjusted ordering number is 18.9.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 [for particulate polycyclic aromatic hydrocarbons (PPAH). This TLV recognizes the carcinogenic potential of PPAH collectively].

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/18.9 = 3.7 \times 10^3$ μg/m^3	Air, Ecology:
Water, Health: $15 \times 3.7 \times 10^3 = 5.55 \times 10^4$ μg/ℓ	Water, Ecology:
Land, Health: $0.2 \times 5.55 \times 10^4 = 1.11 \times 10^4$ μg/g	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 18.9) = 8.8$ μg/m^3

$EPC_{WC} = 15 \times 8.8 = 132$ μg/ℓ

$EPC_{LC} = 0.2 \times 132 = 26.4$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

21D020
DIBENZO(a,h)PYRENE

EMISSION LEVEL GOALS	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			3.7E3		9		
Water, $\mu g/l$ (ppm Wt)			5.55E4		132		
Land, $\mu g/g$ (ppm Wt)			1.1E4		26		

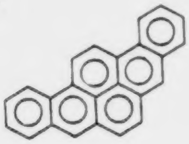
*To be multiplied by dilution factor

AMBIENT LEVEL GOALS	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					9
Water, $\mu g/l$ (ppm Wt)					132
Land, $\mu g/g$ (ppm Wt)					26

WLN: L D6 B66 P666 2AB A+J

CATEGORY: 21D

STRUCTURE:



DIBENZO(a,i)PYRENE: $C_{24}H_{14}$ (benzo(rst)pentaphene; 2,3:6,7-dibenzpyrene; 4,5:8,9-dibenzpyrene). 21D040
Crystallizes as greenish-yellow needles or plates, benzene solutions exhibit blue fluorescence.

PROPERTIES:

Molecular wt: 302.37; mp: 281.5; insoluble in water, solubility may be enhanced by surfactant impurities in water (ref. 1); lipid solubility: 2.5 mg in 0.2 ml tri-octanoin (ref. 4).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Dibenzo(a,i)pyrene is present in coal tar (ref. 5).

Dibenzo(a,i)pyrene is associated with particulate polycyclic aromatic hydrocarbons, PPAH, (ref. 4). The following concentrations of carcinogenic PPAH have been estimated or reported: Air (urban environment in winter in seven selected U.S. cities): 21.6 ng/m^3 - 146 ng/m^3 (ref. 2); ground-water and surface-treated water: 0.001 μg/ℓ - 0.025 μg/ℓ (ref. 1): upper layer of Earth's crust: 100 μg/kg - 1,000 μg/kg (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

Dibenzo(a,i)pyrene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 3).

Dibenzo(a,i)pyrene is reported to cause tumors in mice and hamsters. The EPA/NIOSH ordering number is 3225. The lowest dose to induce a carcinogenic response is reported as 2 mg/kg (ref. 9). The adjusted ordering number is 1612.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 [for particulate polycyclic aromatic hydrocarbons (PPAH). This TLV recognizes the carcinogenic potential of PPAH collectively].

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/1{,}612 = 43.4\ \mu g/m^3$
Water, Health: $15 \times 43.4 = 651\ \mu g/\ell$
Land, Health: $0.2 \times 651 = 130.2\ \mu g/g$

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 1{,}612) = 0.1\ \mu g/m^3$
$EPC_{WC} = 15 \times 0.1 = 1.5\ \mu g/\ell$
$EPC_{LC} = 0.2 \times 1.5 = .3\ \mu g/g$

313<

MULTIMEDIA ENVIRONMENTAL GOALS

XX
21D040
DIBENZO(a,i)PYRENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			4.34E1		0.1		
Water, $\mu g/l$ (ppm Wt)			6.51E2		1.5		
Land, $\mu g/g$ (ppm Wt)			1.30E2		0.3		

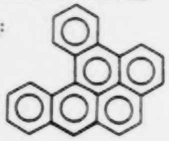
*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					0.1
Water, $\mu g/l$ (ppm Wt)					1.5
Land, $\mu g/g$ (ppm Wt)					0.3

CATEGORY: 21D

WLN: L D66 K666 B6 2AB A&J

STRUCTURE:



DIBENZO(a,l)PYRENE: $C_{24}H_{14}$ (dibenzo(def,p)chrysene; 1,2:9,10-dibenzopyrene; 1,2:3,4-dibenzpyrene; 2,3:4,5-dibenzpyrene) 21D060

Colorless prisms from cyclohexane.

PROPERTIES:

Molecular wt: 302. 37; mp: 164; insoluble in water, solubility may be enhanced by surfactant impurities in water (ref. 1); lipid solubility: 0.6 mg/0.2 ml olive oil (ref. 4).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Dibenzo(a,l)pyrene is probably not a naturally occurring isomer. Its synthesis has been reported (ref. 5). Investigations previous to 1966 concerning dibenzo(a,l)pyrene were probably carried out with dibenzo(a,e)fluoranthene (ref. 5). If the compound occurs in the atmosphere, it will probably be associated with particulate polycyclic aromatic hydrocarbons, PPAH.

TOXIC PROPERTIES, HEALTH EFFECTS:

Dibenzo(a,l)pyrene is reported to cause tumors in mice. The EPA/NIOSH ordering number is 3101. The lowest dose to induce a carcinogenic response is reported as 48 mg/kg (ref. 9). The adjusted ordering number is 64.6.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/64.6 = 1.08 \times 10^3$ μg/m^3

Water, Health: $15 \times 1.08 \times 10^3 = 1.6 \times 10^4$ μg/ℓ

Land, Health: $0.2 \times 1.6 \times 10^4 = 3.2 \times 10^3$ μg/g

Air, Ecology:

Water, Ecology:

Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 64.6) = 2.6$ μg/m^3

$EPC_{WC} = 15 \times 2.6 = 39$ μg/ℓ

$EPC_{LC} = 0.2 \times 39 = 7.8$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

21D060
DIBENZO(a,l)PYRENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			1.1E3		3		
Water, μg/l (ppm Wt)			1.6E4		39		
Land, μg/g (ppm Wt)			3.2E3		8		

*To be multiplied by dilution factor

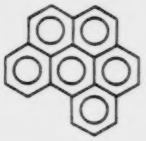
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)					3
Water, μg/l (ppm Wt)					39
Land, μg/g (ppm Wt)					8

CATEGORY: 21D

BENZO(ghi)PERYLENE: $C_{22}H_{12}$ (1,12-Benzoperylene). 21D080
Leaflets from benzene; exhibits bright green-yellow fluorescence.

WLN: L666 B6 C6 D6 4ABCD VJ

STRUCTURE:



PROPERTIES:

Molecular wt: 276.33; mp: 222-3; insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzo(ghi)perylene occurs in tar and in smoke-polluted atmospheres. The urban concentration for benzo(ghi)perylene is reported as 3.27 ng/m^3 (ref. 6).

Benzo(ghi)perylene is associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 2). The following concentrations of carcinogenic PPAH have been estimated or reported: Air (urban environment in winter in seven selected U.S. cities): 21.6 ng/m^3 - 146 ng/m^3 (ref. 2); ground-water and surface-treated water: 0.001 μg/ℓ - 0.025 μg/ℓ (ref. 1): upper layer of earth's crust: 100 μg/kg - 1,000 μg/kg (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

Benzo(ghi)perylene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Topical application of benzo(ghi)perylene in acetone solution (mixture with phenanthrene, anthracene, pyrene, fluoranthene, chrysene, 3,4- and 1,2-benzopyrene, 1,2,5,6-dibenzanthracene, and 1,2-benzanthracene) induced four tumors in 225 mice (ref. 7). Data pertinent to the carcinogenic potential of benzo(ghi)perylene alone are currently not available. The compound is probably not a highly active carcinogen.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Benzo(ghi)perylene appears on EPA Consent Decree List with an assigned priority of 1.

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	Air, Ecology:
Water, Health:	Water, Ecology:
Land, Health:	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

21D080
BENZO(ghi)PERYLENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							0.003+
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

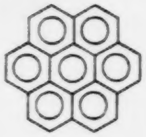
+ Value Is For Urban Atmosphere. No Rural Concentration Is Reported.

CATEGORY: 21D

WLN: L666 B6 C6 D6 E6 6ABCDEF A&J

CORONENE: $C_{24}H_{12}$ (hexabenzobenzene). 21D100

STRUCTURE:



Yellow needles from benzene; solutions exhibit bluish-violet fluorescence.

PROPERTIES:

Molecular wt: 300.36; mp: 438; bp: 525; d: 1.377; insoluble in water, solubility may be enhanced by surfactant impurities in water (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Urban concentrations of coronene are reported ranging from 1.252 ng/1,500 m^3 to 2.13 ng/m^3 (ref. 6).

Coronene is associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 2). The following concentrations of carcinogenic PPAH have been estimated or reported: Air (urban environment in winter in seven selected U.S. cities): 21.6 ng/m^3 - 146 ng/m^3 (ref. 2); ground-water and surface-treated water: 0.001 μg/ℓ - 0.025 μg/ℓ (ref. 1): upper layer of earth's crust: 100 μg/kg - 1,000 μg/kg (ref. 1).

It has also been identified in estuarine soils and in the mineral curtisite (ref. 8).

TOXIC PROPERTIES, HEALTH EFFECTS:

Coronene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Topical application of coronene in acetone solution (mixture with phenanthrene, anthracene, pyrene, fluoranthene, chrysene, 3,4- and 1,2-benzopyrene, 1,12-benzperylene, anthanthrene, 1,2,5,6-dibenzanthracene, and 1,2-benzanthracene) induced four tumors in 225 mice (ref. 7). Data pertinent to the carcinogenic potential of coronene alone are currently unavailable.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:
Water, Health:
Land, Health:

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

21D100
CORONENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							8.0×10^{-7} to + 2.13×10^{-6}
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

+ Value For Urban Concentration Is Reported. No Rural Concentration Is Reported.

REFERENCES: CATEGORY 21D

Fused Polycyclic Hydrocarbons - Compounds with More Than Five Fused Rings

1. Andelman, J. B., and M. J. Suess. Polynuclear Aromatic Hydrocarbons in the Water Environment. Bull Wld. Hlth. Org. 43: 479-508 (1970).

2. U.S. Environmental Protection Agency, Office of Research and Development. Scientific and Technical Assessment Report on Particulate Polycyclic Organic Matter (PPOM). Star Series. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC EPA-600/6-74-001 (1975).

3. Searle, C. E., Ed. Chemical Carcinogens. ACS Monograph 173. American Chemical Society, Washington, DC (1976).

4. National Cancer Institute. Survey of Compounds Which Have Been Tested for Carcinogenic Activity: 1961-1967 Volume. Prepared by John I. Thompson and Co., Rockville, MD under Contract No. NIH-69-2086 for National Cancer Institute. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC. Public Health Service Publication No. 149.

5. International Agency for Research on Cancer. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Man, Vol. 3, Lyon, France. A World Health Organization Publication (WHO), Geneva (1973).

6. Wagoner, D. Compilation of Ambient Trace Substances. Draft of Report Prepared by Research Triangle Institute Under Contract No. 68-02-1325 for U.S. Environmental Protection Agency. Available from W. G. Tucker, Project Officer, IERL-EPA, Research Triangle Park, N.C. (1976).

7. National Cancer Institute. Survey of Compounds Which Have Been Tested for Carcinogenic Activity: 1972-1973 Volume. Prepared by Tracor Jitco Inc., Rockville, MD under Contract No. 1 CP 33402 for National Cancer Institute. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC. Public Health Service Publication No. 149.

8. Kingsbury, G. L., R. C. Sims, and J. B. White. Source and Ambient Concentration Data for Polycyclic Organic Matter. Vol. I-III. Draft of Report Prepared by Research Triangle Institute, under Contract No. 68-02-2612 for U.S. Environmental Protection Agency. Available from J. O. Milliken, Project Officer, IERL-EPA, Research Triangle Park, N.C. (1978).

9. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared for Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

CATEGORY 22

FUSED NON-ALTERNANT POLYCYCLIC HYDROCARBONS

SUBCATEGORY: 22A - Two- and Three-Ring Fused Non-Alternant Polycyclic Hydrocarbons

Summary of Subcategory

Total number of compounds in subcategory	3
number of parent compounds with subspecies	0
number of subspecies	0
Number of parent compounds with no MEG values	2
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

Consent Decree compounds included in subcategory: 1

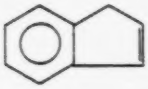
22A020 Fluorene

CATEGORY: 22A

WLN: L56 BHJ

INDENE: C_9H_8 (indonaphthene).
A colorless liquid. 22A010

STRUCTURE:



PROPERTIES:

Molecular wt: 116.16; mp: -1.8; bp: 181.6; d: 0.996;
insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Indene is found in coal tar.

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{Lo} (subcutaneous, rat): 1,000 mg/kg.

Serious systemic responses may result from exposure to high concentrations of indene absorbed primarily through inhalation (ref. 2).

The epoxide is considered inactive as a skin carcinogen in animals (ref. 3).

Indene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 3).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 45 mg/m^3 (10 ppm).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 4.5×10^4 $\mu g/m^3$ (10 ppm)	Air, Ecology:
Water, Health: $15 \times 4.5 \times 10^4 = 6.75 \times 10^5$ $\mu g/\ell$	Water, Ecology:
Land, Health: $0.2 \times 6.75 \times 10^5 = 1.35 \times 10^5$ $\mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 45/420 = 107\ \mu g/m^3$
$EPC_{AH1a} = 10/420 = 0.024$ ppm
$EPC_{WH1} = 15 \times 107 = 1,605\ \mu g/\ell$
$EPC_{WH2} = 13.8 \times 45 = 621\ \mu g/\ell$
$EPC_{LH} = 0.2 \times 621 = 120\ \mu g/g$

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			4.5E4 (10)		107 (0.024)		
Water, $\mu g/l$ (ppm Wt)			6.75E5		621		
Land, $\mu g/g$ (ppm Wt)			1.4E5		120		

*To be multiplied by dilution factor

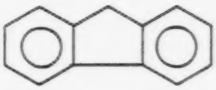
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			107 (0.024)		
Water, $\mu g/l$ (ppm Wt)			621		
Land, $\mu g/g$ (ppm Wt)			120		

CATEGORY: 22A

WLN:

FLUORENE: $C_{13}H_{10}$ (2,3-benzindene, diphenylenemethane). 22A020
Fluorescent, colorless flakes.

STRUCTURE:



PROPERTIES:

Molecular$_0$wt: 166.15; mp: 116-117; bp: 293-295; d: 1.203^0; vap. p: 10 mm at 146.0°C; insoluble in water, solubility may be enhanced by surfactant impurities in water (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Fluorene is among the lower molecular weight polycyclic hydrocarbons comprising the volatile portion of the benzene soluble fraction of coal tar (ref. 2). Fluorene is associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 4). The following concentrations of PPAH have been estimated or reported: Air (urban environment in winter in seven selected U.S. cities): 21.6 ng/m^3 - 146 ng/m^3 (ref. 4); groundwater and surface-treated water: 0.001 μg/ℓ - 0.025 μg/ℓ (ref. 1): upper layer of earth's crust: 100 μg/kg - 1,000 μg/kg (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

Fluorene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Carcinogenic polycyclic aromatic hydrocarbons may induce tumors at the site of application (ref. 3). There is currently no evidence to indicate that fluorene alone is carcinogenic.

Subcutaneous injection of fluorene in a 1:1 molar ratio to benzo(a)pyrene showed no inhibitory effect on the carcinogenicity of B(a)P (ref. 5).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Fluorene appears on EPA Consent Decree List with an assigned priority of 1.

TLV (coal tar pitch volatiles): 0.2 mg/m^3.

[The specification includes naphthalene, anthracene, acridine, phenanthrene, and fluorene, collectively. The purpose of the TLV is to minimize concentrations of higher weight polycyclic hydrocarbons which are carcinogenic (ref. 2).]

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	Air, Ecology:
Water, Health:	Water, Ecology:
Land, Health:	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

22A020
FLUORENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, µg/m^3 (ppm Vol)							
Water, µg/l (ppm Wt)							
Land, µg/g (ppm Wt)							

*To be multiplied by dilution factor

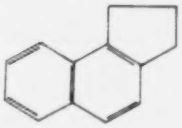
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, µg/m^3 (ppm Vol)					
Water, µg/l (ppm Wt)					
Land, µg/g (ppm Wt)					

CATEGORY: 22A

WLN:

CYCLOPENTANONAPHTHALENE: $C_{13}H_{12}$.
(1,2-cyclopentano-naphthalene, 4,5-benzindane). 22A040
A colorless liquid.

STRUCTURE:



PROPERTIES:

Molecular wt: 168.24 ; bp: $294\text{-}5^{757}$; d: 1.066^{20}_{4}; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

The compound may occur as a constituent of particulate polycyclic aromatic hydrocarbons, PPAH. It is present in coal tar in the 290-300° fraction (ref. 6).

TOXIC PROPERTIES, HEALTH EFFECTS:

Certain polycyclic aromatic hydrocarbons, when administered topically to animals, may induce tumors at the site of application (ref. 3).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m³ (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

22A040
CYCLOPENTANONAPHTHALENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

REFERENCES: CATEGORY 82A

Fused Non-Alternant Polycyclic Hydrocarbons - Two- and Three-Ring Fused Non-Alternant Polycyclic Hydrocarbons

1. Andelman, J. B., and M. J. Suess. Polynuclear Aromatic Hydrocarbons in the Water Environment. *Bull Wld. Hlth. Org.* 43: 479-508 (1970).

2. American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values for Substances in Workroom Air with Supplements, Third Edition. American Conference of Governmental Industrial Hygienists, Cincinnati, OH (1974).

3. Searle, C. E., Ed. Chemical Carcinogens. ACS Monograph 173. American Chemical Society, Washington, DC (1976).

4. U.S. Environmental Protection Agency, Office of Research and Development. Scientific and Technical Assessment Report on Particulate Polycyclic Organic Matter (PPOM). Star Series. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC EPA-600/6-74-001 (1975).

5. National Cancer Institute. Survey of Compounds Which Have Been Tested for Carcinogenic Activity: 1961-1962 Volume. Prepared by John I. Thompson and Co., Rockville, MD under Contract No. NIH-69-2086 for National Cancer Institute. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC. Public Health Service Publication No. 149.

6. Josephy, E., and F. Radt. Elsevier's Encyclopedia of Organic Chemistry, Vol. 13, Elsevier Publishing Co., Inc. (1940).

CATEGORY 22

FUSED NON-ALTERNANT POLYCYCLIC HYDROCARBONS

SUBCATEGORY: 22B - Four Ring Fused Non-Alternant Polycyclic Hydrocarbons

Summary of Subcategory

Total number of compounds in subcategory	4
number of parent compounds with subspecies	0
number of subspecies	0
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	2
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	1

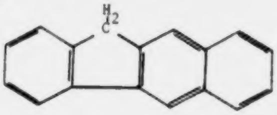
Consent Decree compounds included in subcategory: 1

22B040 Fluoranthene

CATEGORY: 22B
2,3-BENZOFLUORENE: $C_{17}H_{12}$
(benzo(b)fluorene, 11-H benzo(b)fluorene). 22B020
Colorless crystals.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 216.29; mp: 208-9; bp: 401-2; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

2,3-Benzofluorene has been reported in urban atmosphere at a concentration of 4.587 µg/1,500 m^3 (ref. 1). It is associated with particulate polycyclic aromatic hydrocarbons (ref. 2). The compound occurs in coal tar pitch (ref. 3).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for 2,3-benzofluorene are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

22B020
2,3-BENZOFLUORENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)							3.05×10^{-3} †
Water, μg/l (ppm Wt)							
Land, μg/g (ppm Wt)							

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)					
Water, μg/l (ppm Wt)					
Land, μg/g (ppm Wt)					

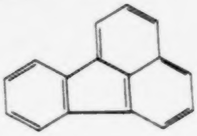
† Value For Urban Atmosphere Is Reported. No Rural Concentration Is Reported.

CATEGORY: 22B

WLN: L C6566 1A PJ

FLUORANTHENE: $C_{16}H_{10}$ (benzo(j,k)fluorene). 22B040
Colorless needles or plates from alcohol.

STRUCTURE:



PROPERTIES:

Molecular wt: 202.26; mp: 110; insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 4).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Fluoranthene is present in coal tar (ref. 5) and is associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 2). The following concentrations of PPAH have been estimated or reported: Air (urban environment in winter in seven selected U.S. cities): 21.6 ng/m^3 - 146 ng/m^3 (ref. 2); ground-water and surface-treated water: 0.001 μg/ℓ - 0.025 μg/ℓ (ref. 4): upper layer of earth's crust: 100 μg/kg - 1,000 μg/kg (ref. 4).

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{50} (oral, rat): 2,000 mg/kg

Fluoranthene may be present in soot, coal tar, and pitch which are known to be carcinogenic to man. Topical application of fluoranthene in acetone (mixture with phenanthrene, anthracene, pyrene, chrysene, B(a)P, B(e)P, perylene, anthanthrene, DB(a,j)A, and BA) induced four tumors in 225 mice (ref. 6). There is currently no evidence to indicate that fluoranthene alone is carcinogenic.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

Fluoranthene appears on the EPA Consent Decree List with an assigned priority of 2.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 45 x 2,000 = 9.0×10^4 μg/m^3	Air, Ecology:
Water, Health: 15 x 9 x 10^4 = 1.4×10^6 μg/ℓ	Water, Ecology:
Land, Health: 0.2 x 1.4 x 10^6 = 2.8×10^5 μg/g	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

EPC_{AH2} = 0.107 x 2,000 = 214 μg/m^3
EPC_{AH3} = 0.081 x 2,000 = 162 μg/m^3
EPC_{WH1} = 15 x 162 = 2,430 μg/ℓ
EPC_{WH2} = 0.4 x 2,000 = 800 μg/ℓ
EPC_{LH} = 0.2 x 800 = 160 μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

22B040
FLUORANTHENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			9.0E4		162		
Water, $\mu g/l$ (ppm Wt)			1.4E6		800		
Land, $\mu g/g$ (ppm Wt)			2.8E5		160		

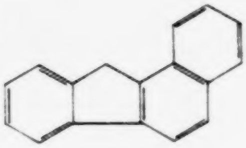
*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			162		
Water, $\mu g/l$ (ppm Wt)			800		
Land, $\mu g/g$ (ppm Wt)			160		

CATEGORY: 22B
1,2-BENZOFLUORENE: $C_{17}H_{12}$
(chrysofluorene, benzo(a)fluorene, 11-H benzo(a)fluorene).
A solid. 22B060

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 216.29; mp: 189-90; bp: 413^{760}

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

1,2-Benzofluorene has been reported in urban atmosphere at a concentration of 2.557 μg/1,500 m^3 (ref. 1). The compound occurs as a constituent of particulate polycyclic aromatic hydrocarbons, PPAH (ref. 2). The compound has also been reported in samples taken from river water (ref. 7).

TOXIC PROPERTIES, HEALTH EFFECTS:

Certain polycyclic aromatic hydrocarbons when administered topically to animals may induce tumors at the site of application (ref. 4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

22B060
1,2-BENZOFLUORENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							$1.70 \text{x} 10^{-3}$†
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

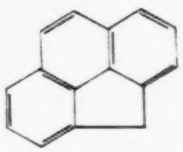
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

† Value For Urban Atmoshpere Is Reported. No Rural Concentration Is Reported.

CATEGORY: 22B
CYCLOPENTA(def)PHENANTHRENE: $C_{15}H_{10}$ 22B080
(4H-cyclopenta(def)phenanthrene, phenanthrylene methane)
Crystalline leaflets.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 190.080; mp: 116; bp: 353^{760}; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Cyclopenta(def)phenanthrene is reported to occur in coal tar (ref. 3). It and its methyl dimethyl and ethyl derivatives have been identified in ambient urban air samples taken in Indiana (ref. 11).

TOXIC PROPERTIES, HEALTH EFFECTS:

Cyclopenta(def)phenanthrene has been found to cause cancer in rats (ref. 8). The lowest reported dosage to induce cancer is 3,000 mg/kg. The EPA/NIOSH ordering number is 4,111 and the adjusted ordering number is 1.37.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$7 \times 10^4/1.37 = 5.11 \times 10^4$ μg/m^3	Air, Ecology:
Water, Health:	$15 \times 5.11 \times 10^4 = 7.67 \times 10^5$ μg/l	Water, Ecology:
Land, Health:	$0.2 \times 7.67 \times 10^5 = 1.5 \times 10^5$ μg/g	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 1.37) = 121.7$ μg/m^3

$EPC_{WC} = 15 \times 121.7 = 1,826$ μg/l

$EPC_{LC} = 0.2 \times 1,826 = 365$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

22B080
CYCLOPENTA(def)PHENANTHRENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			5.1E4		122		
Water, $\mu g/l$ (ppm Wt)			7.7E5		1,826		
Land, $\mu g/g$ (ppm Wt)			1.5E5		365		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					122
Water, $\mu g/l$ (ppm Wt)					1,826
Land, $\mu g/g$ (ppm Wt)					365

REFERENCES: CATEGORY 22B

Fused Non-Alternant Polycyclic Hydrocarbons -
Four Ring Fused Non-Alternant Polycyclic Hydrocarbons

1. Wagoner, D. Compilation of Ambient Trace Substances. Draft of Report Prepared by Research Triangle Institute Under Contract No. 68-02-1325 for U.S. Environmental Protection Agency. Available from W. G. Tucker, Project Officer, IERL-EPA, Research Triangle Park, N.C. (1976).

2. U.S. Environmental Protection Agency, Office of Research and Development. Scientific and Technical Assessment Report on Particulate Polycyclic Organic Matter (PPOM). Star Series. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC EPA-600/6-74-001 (1975).

3. Josephy, E., and F. Radt. Elsevier's Encyclopedia of Organic Chemistry, Vol. 14, Elsevier Publishing Co. Inc. (1940).

4. Andelman, J. B., and M. J. Suess. Polynuclear Aromatic Hydrocarbons in the Water Environment. Bull Wld. Hlth. Org. 43: 479-508 (1970).

5. Clar, E. J. Polycyclic Hydrocarbons. Academic Press, London (1964).

6. National Cancer Institute. Survey of Compounds Which Have Been Tested for Carcinogenic Activity: 1972-1973 Volume. Prepared by Tracor Jitco Inc., Rockville, MD under Contract No. 1 CP 33402 for National Cancer Institute. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC. Public Health Service Publication No. 149.

7. Shackelford, W. M., and L. H. Keith. Frequency of Organic Compounds Identified in Water. EPA Publication No. 600/4/76-062, December 1976.

8. Braunstein, H. M., E. D. Copenhauer, and H. A. Pfuderer (Eds.). Environmental, Health, and Control Aspects of Coal Conversion: An Information Overview. Oak Ridge National Laboratory, Oak Ridge, TN 37830. Prepared for the Energy Research and Development Administration Assistant Administration for Environmental Safety, April 1977.

9. National Cancer Institute. Survey of Compounds Which Have Been Tested for Carcinogenic Activity: 1961-1967 Volume. Prepared by John I. Thompson and Co., Rockville, MD under Contract No. NIH-69-2086 for National Cancer Institute. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC. Public Health Service Publication No. 149.

10. International Agency for Research on Cancer. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Man, Vol. 3, Lyon, France. A World Health Organization Publication (WHO), Geneva (1973).

REFERENCES: CATEGORY 22B (Continued)

11. Kingsbury, G. L., R. C. Sims, and J. B. White. Source and Ambient Concentration Data for Polycyclic Organic Matter. Vol. I-III. Draft of Report Prepared by Research Triangle Institute, under Contract No. 68-02-2612 for U.S. Environmental Protection Agency. Available from J. O. Milliken, Project Officer, IERL-EPA, Research Triangle Park, N.C. (1978).

CATEGORY 22

FUSED NON-ALTERNANT POLYCYCLIC HYDROCARBONS

SUBCATEGORY: 22C - Five Ring Fused Non-Alternant Polycyclic Hydrocarbons

Summary of Subcategory

Total number of compounds in subcategory	4
number of parent compounds with subspecies	0
number of subspecies	0
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	3

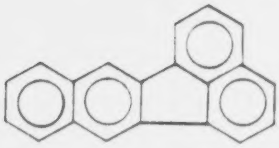
Consent Decree compounds included in subcategory: 2

22C020	Benzo(k)fluoranthene
22C080	Benzo(b)fluoranthene

CATEGORY: 22C
BENZO(K)FLUORANTHENE: $C_{20}H_{12}$ 22C020
(11,12-benzofluoranthene; 8,9-benzfluoranthene).
A crystal.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 252.32; mp: 217; bp: 480^{760}; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzo(k)fluoranthene has been reported in urban atmosphere at a concentration of 0.0002 µg/m³ (ref. 1). The compound occurs as a constituent of particulate polycyclic aromatic hydrocarbons, PPAH (ref. 2). The compound has also been reported in samples taken from river water, ground water, and finished drinking water (ref. 3). Benzo(k)fluoranthene has been reported to be present in foods (raw and cooked) (ref. 4).

TOXIC PROPERTIES, HEALTH EFFECTS:

Benzo(k)fluoranthene gives a consistent carcinogenic response in experimental animals (ref. 4). The lowest dose to induce a carcinogenic response in animals is 72 mg/kg (ref. 7). The EPA/NIOSH ordering number is 3,122 and the adjusted ordering number is 43.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m³ (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

Benzo(k)fluoranthene is on the EPA Consent Decree Priority 1 List.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$7 \times 10^4/43 = 1{,}628$ µg/m³	Air, Ecology:
Water, Health:	$15 \times 1{,}628 = 2.44 \times 10^4$ µg/l	Water, Ecology:
Land, Health:	$0.2 \times 2.44 \times 10^4 = 4.88 \times 10^3$	µg/g Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 43) = 3.88$ µg/m³

$EPC_{WC} = 15 \times 3.88 = 58.2$ µg/l

$EPC_{LC} = 0.2 \times 58.2 = 11.64$ µg/g

MULTIMEDIA ENVIRONMENTAL GOALS

22C020
BENZO(k)FLUORANTHENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			1.6E3		3.9		.0002†
Water, μg/l (ppm Wt)			2.4E4		58		
Land, μg/g (ppm Wt)			4.9E3		11.7		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)					3.9
Water, μg/l (ppm Wt)					58
Land, μg/g (ppm Wt)					11.7

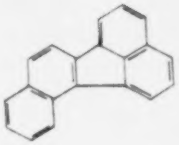
† Urban concentration. Rural concentration not available.

CATEGORY: 22C

WLN: L D6 C6566 1A TJ

BENZO(j)FLUORANTHENE: $C_{20}H_{12}$ (10,11-benzofluoranthene; B(j)F; 7,8-benzfluoranthene). 22C040
Yellow plates or needles from alcohol.

STRUCTURE:



PROPERTIES:

Molecular wt: 252.32; mp: 165; insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 5).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzo(j)fluoranthene may be obtained from coal tar and from the high-temperature pyrolysis of anthracene, naphthalene, tobacco constituents, and other organic compounds (ref. 6). A concentration of B(j)F in urban atmosphere is reported as 1.3 ng/m^3 (ref. 1). Benzo(j)fluoranthene is associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 2). Other environmental concentrations of B(j)F (with B(b)F) are reported as follows: soil--15 to 110 μg/kg; drinking water--1 to 14.0 $\mu g/m^3$ (ref. 6). It has also been detected in oils of certain fruits and in cooked foods (ref. 6).

TOXIC PROPERTIES, HEALTH EFFECTS:

Benzo(j)fluoranthene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Benzo(j)fluoranthene is reported to cause tumors in mice. The EPA/NIOSH ordering number is 3121. The lowest dose to induce a carcinogenic response is reported as 288 mg/kg (ref. 7). The adjusted ordering number of 10.8

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/10.8 = 6.5 \times 10^3\ \mu g/m^3$
Water, Health: $15 \times 6.5 \times 10^3 = 9.8 \times 10^4\ \mu g/\ell$
Land, Health: $0.2 \times 9.8 \times 10^4 = 1.96 \times 10^4\ \mu g/g$

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 10.8) = 15.4\ \mu g/m^3$
$EPC_{WC} = 15 \times 15.4 = 231\ \mu g/\ell$
$EPC_{LC} = 0.2 \times 231 = 46.2\ \mu g/g$

22C040
BENZO(j)FLUORANTHENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			6.5E3		15		0.001†
Water, $\mu g/l$ (ppm Wt)			9.8E4		231		
Land, $\mu g/g$ (ppm Wt)			1.96E4		46		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			15		
Water, $\mu g/l$ (ppm Wt)			231		
Land, $\mu g/g$ (ppm Wt)			46		

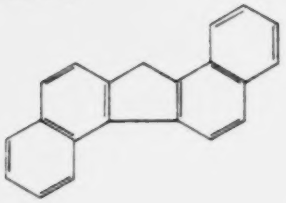
† Reported For Urban Atmosphere. No Rural Concentration is Reported.

CATEGORY: 22C

1,2:5,6-DIBENZO FLUORENE: $C_{21}H_{14}$ 22C060
(13H-dibenzo(a,g)fluorene).
A solid.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt:266.35; mp:174-5; bp:195-200; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

The compound occurs as a constituent of particulate polycyclic aromatic hydrocarbons, PPAH (ref. 2).

TOXIC PROPERTIES, HEALTH EFFECTS:

1,2:5,6-dibenzofluorene has been shown to induce a carcinogenic response when administered to experimental animals (ref. 8). The lowest dose to induce cancer is reported to be 590 mg/kg (ref. 7). The EPA/NIOSH ordering number is 3,121 and the adjusted ordering number is 5.29.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$7 \times 10^4/5.29 = 1.32 \times 10^4$ $\mu g/m^3$	Air, Ecology:
Water, Health:	$15 \times 1.32 \times 10^4 = 1.98 \times 10^5$ $\mu g/l$	Water, Ecology:
Land, Health:	$0.2 \times 1.98 \times 10^5 = 3.96 \times 10^4$ $\mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 5.29) = 31.5$ $\mu g/m^3$

$EPC_{WC} = 15 \times 31.5 = 472.5$ $\mu g/l$

$EPC_{LC} = 0.2 \times 472.5 = 94.5$ $\mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

22C060
1,2:5,6-DIBENZO FLUORENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			1.3E4		31.5		
Water, μg/l (ppm Wt)			2.0E5		472		
Land, μg/g (ppm Wt)			4.0E4		94.5		

*To be multiplied by dilution factor

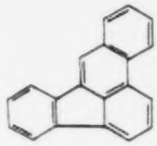
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)					31.5
Water, μg/l (ppm Wt)					472
Land, μg/g (ppm Wt)					94.5

CATEGORY: 22C

WLN: L C65 K666 1A

BENZO(b)FLUORANTHENE: $C_{20}H_{12}$ (benz(e)acephenantrylene, 2,3-benzofluoranthene, B(b)F). 22C080
Needles from benzene.

STRUCTURE:



PROPERTIES:

Molecular wt: 252.32; mp: 167; insoluble in water; solubility may be enhanced by surfactant impurities in water (ref. 4); lipid solubility: 0.6 mg/2 ml olive oil (ref. 9).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzo(b)fluoranthene is formed by the high-temperature pyrolysis of anthracene, some tobacco constituents, and other organic compounds (ref. 10). Benzo(b)fluoranthene is associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 2). Concentrations of benzo(b)fluoranthene measured in urban atmosphere range from 0.54 ng/m^3 to 22 ng/m^3 (ref. 1). Other environmental concentrations of B(b)F with B(j)F are reported as follows: drinking water--0.8 to 11.5 μg/m^3; soils (nonindustrial)--15 to 110 μg/kg (ref. 10). It has also been detected in foods, leaves of various trees, and algae (ref. 10).

TOXIC PROPERTIES, HEALTH EFFECTS:

Benzo(b)fluoranthene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Benzo(b)fluoranthene is reported to produce tumors in mice. The EPA/NIOSH ordering number is 3122. The lowest dose to induce a carcinogenic response is reported as 40 mg/kg (ref. 7). The adjusted ordering number is 78.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Benzo(b)fluoranthene appears on EPA Consent Decree List with an assigned priority of 1.

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/78 = 900$ μg/m^3
Water, Health: $15 \times 900 = 1.34 \times 10^4$ μg/ℓ
Land, Health: $0.2 \times 1.34 \times 10^4 = 2.68 \times 10^3$ μg/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 78) = 2.1$ μg/m^3
$EPC_{WC} = 15 \times 2.1 = 31.5$ μg/ℓ
$EPC_{LC} = 0.2 \times 31.5 = 6.3$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

22C080
BENZO(b)FLUORANTHENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			9.0E2		2.1		0.0005-0.02†
Water, $\mu g/l$ (ppm Wt)			1.3E4		31.5		
Land, $\mu g/g$ (ppm Wt)			2.7E3		6.3		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					2.1
Water, $\mu g/l$ (ppm Wt)					31.5
Land, $\mu g/g$ (ppm Wt)					6.3

† Reported For Urban Atmosphere. No Rural Concentration Is Reported.

REFERENCES: CATEGORY 22C

Fused Non-Alternant Polycyclic Hydrocarbons - Five Ring Fused Non-Alternant Polycyclic Hydrocarbons

1. Wagoner, D. Compilation of Ambient Trace Substances. Draft of Report Prepared by Research Triangle Institute Under Contract No. 68-02-1325 for U.S. Environmental Protection Agency. Available from W. G. Tucker, Project Officer, IERL-EPA, Research Triangle Park, N.C. (1976).

2. U.S. Environmental Protection Agency, Office of Research and Development. Scientific and Technical Assessment Report on Particulate Polycyclic Organic Matter (PPOM). Star Series. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC EPA-600/6-74-001 (1975).

3. Shackelford, W. M., and L. H. Keith. Frequency of Organic Compounds Identified in Water. EPA Publication No. 600/4-76-062, December 1976.

4. Searle, C. E., Ed. Chemical Carcinogens. ACS Monograph 173. American Chemical Society, Washington, DC (1976).

5. Andelman, J. B., and M. J. Suess. Polynuclear Aromatic Hydrocarbons in the Water Environment. Bull Wld. Hlth. Org. 43: 479-508 (1970).

6. International Agency for Research on Cancer. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Man, Vol. 3, Lyon, France. A World Health Organization Publication (WHO), Geneva (1973).

7. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco, Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

CATEGORY 22D

FUSED NON-ALTERNANT POLYCYCLIC HYDROCARBONS

SUBCATEGORY: 22D - Compounds with More than Five Fused Rings

Summary of Subcategory

Total number of compounds in subcategory	2
number of parent compounds with subspecies	0
number of subspecies	0
Number of parent compounds with no MEG values	1
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	1

Consent Decree compounds included in subcategory: 1

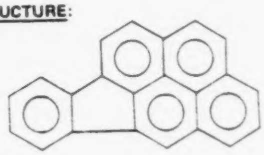
22D020 Indeno(1,2,3-cd)pyrene

CATEGORY: 22D

WLN: L E6 C5666 B6 3ABC BJ

INDENO(1,2,3-cd)PYRENE: $C_{22}H_{12}$ (2,3-o-phenylenepyrene, IP). Yellow plates or needles from light petroleum, greenish fluorescence. 22D020

STRUCTURE:



PROPERTIES:

Molecular wt: 276.34; mp: 162.5-164; insoluble in water; solubility may be enhanced by surfactant impurities in water; lipid solubility: 0.6 mg/2 ml olive oil (ref. 1).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Indeno(1,2,3-cd)pyrene is present in coal tar. It is formed by high-temperature pyrolysis of tobacco constituents (ref. 2). Indeno(1,2,3-cd)pyrene is associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 3). Environmental concentrations of indeno(1,2,3-cd)pyrene are reported as follows: air dust--0.96 mg/kg; soils (forest)--0.6 mg/kg; drinking water--0.1 to 12.6 $\mu g/m^3$ (ref. 2). It has also been detected in oils from certain fruits, leaves of various kinds of trees, and in algae (ref. 2).

TOXIC PROPERTIES, HEALTH EFFECTS:

Indeno(1,2,3-cd)pyrene may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man. Indeno(1,2,3-cd)pyrene is reported to cause tumors in mice. The EPA/NIOSH ordering number is 3101. The lowest dose to induce a carcinogenic response is reported as 72 mg/kg (ref. 4). The adjusted ordering number is 43.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

Indeno(1,2,3-cd)pyrene appears on EPA Consent Decree List with an assigned priority of 1.

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/43 = 1.63 \times 10^3\ \mu g/m^3$

Water, Health: $15 \times 1.63 \times 10^3 = 2.4 \times 10^4\ \mu g/\ell$

Land, Health: $0.2 \times 2.4 \times 10^4 = 4.8 \times 10^3\ \mu g/g$

Air, Ecology:

Water, Ecology:

Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 43) = 3.9\ \mu g/m^3$

$EPC_{WC} = 15 \times 3.9 = 58.5\ \mu g/\ell$

$EPC_{LC} = 0.2 \times 58.5 = 11.7\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

22D020
INDENO(1,2,3-cd)PYRENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)			1.63E3		3.9		
Water, μg/l (ppm Wt)			2.4E4		58.5		0.0001-01 †
Land, μg/g (ppm Wt)			4.8E3		11.7		0.6

*To be multiplied by dilution factor

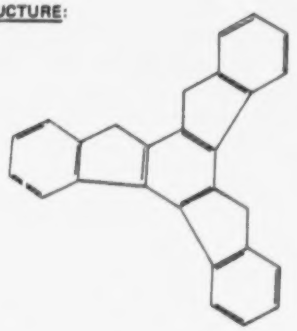
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)					3.9
Water, μg/l (ppm Wt)					58.5
Land, μg/g (ppm Wt)					11.7

† Drinking Water

CATEGORY: 22D
TRIBENZYLENE BENZENE: $C_{27}H_{18}$ 22D040
(truxene).
A solid showing yellow fluorescence.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 342.44; mp: 365-8; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for tribenzylene benzene are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

22D040
TRIBENZYLENE BENZENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

REFERENCES: CATEGORY 22D

Fused Non-Alternant Polycyclic Hydrocarbons -
Compounds with More Than Five Fused Rings

1. National Cancer Institute. Survey of Compounds Which Have Been Tested for Carcinogenic Activity: 1961-1962 Volume. Prepared by John I. Thompson and Co., Rockville, MD under Contract No. NIH-69-2086 for National Cancer Institute. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC. Public Health Service Publication No. 149.

2. International Agency for Research on Cancer. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Man, Vol. 3, Lyon, France. A World Health Organization Publication (WHO), Geneva (1973).

3. U.S. Environmental Protection Agency, Office of Research and Development. Scientific and Technical Assessment Report on Particulate Polycyclic Organic Matter (PPOM). Star Series. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC EPA-600/6-74-001 (1975).

4. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication (NIOSH) 76-191 (1976).

CATEGORY 23

HETEROCYCLIC NITROGEN COMPOUNDS

SUBCATEGORY: 23A - Pyridine and Substituted Pyridines

Summary of Subcategory

Total number of compounds in subcategory	22
number of parent compounds with subspecies	6
number of subspecies	21
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

Consent Decree compounds included in subcategory: 0

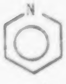
357<

CATEGORY: 23A

WLN: T6NJ

PYRIDINE: C_5H_5N (azabenzene, azine). 23A020
Colorless liquid; sharp, penetrating odor, burning taste.

STRUCTURE:



PROPERTIES:

Molecular wt: 79.10; mp: -42; bp: 115.5; d: 0.9819^{20};
vap. press: 10 mm at 13.2° C; vap. d: 2.73; pK_a: 5.23 (ref. 1); soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Pyridine and its methyl derivatives are usually obtained from the degradation of coal. As a typical heterocyclic aromatic compound, pyridine undergoes both nucleophilic and electrophilic substitutions. Pyridine is photolytically active (ref. 2). The basicity of pyridine is less than that of aromatic amines (ref. 3).

The odor threshold for pyridine is reported as 0.021 ppm or approximately 68 $\mu g/m^3$ (ref. 4). The rural concentration of pyridine is reported as 21 ppb (ref. 5). This is equivalent to 67.7 $\mu g/m^3$. (This level is probably high since it is representative of an agricultural area.)

TOXIC PROPERTIES, HEALTH EFFECTS:

Pyridine is mildly irritating to the skin and causes depression of the central nervous system. Mild symptoms are reported from exposure to 10 ppm. Chronic poisoning may result in damage to liver, kidney, and bone marrow (ref 6).

LD_{50} (oral, rat): 891 mg/kg.
LC_{50} (inhalation, rat): 4,000 ppm for 4 hr.
Toxicity to aquatic life: The 96-hr TLm is reported ranging from 1,000 to 100 ppm (ref. 7).
Pyridine in water in concentrations as low as 5 mg/ℓ may cause tainting of fish flesh (refs. 8,9).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 15 mg/m^3 (5 ppm). (The TLV is sufficient to prevent acute or chronic poisoning but is substantially higher than the odor threshold.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 1.50×10^4 $\mu g/m^3$ (5 ppm)
Water, Health: $15 \times 1.50 \times 10^4 = 2.25 \times 10^5$ $\mu g/\ell$
Land, Health: $0.2 \times 2.25 \times 10^5 = 4.5 \times 10^4$ $\mu g/g$

Air, Ecology:
Water, Ecology: $100 \times 100 = 1.0 \times 10^4$ $\mu g/\ell$
Land, Ecology: $0.2 \times 1.0 \times 10^4 = 2{,}000$ $\mu g/g$

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 10^3 \times 15/420 = 35.7$ $\mu g/m^3$
$EPC_{AH1a} = 5/420 = 0.012$ ppm
$EPC_{WH1} = 15 \times 35.7 = 535.5$ $\mu g/\ell$
$EPC_{WH2} = 13.8 \times 15 = 207$ $\mu g/\ell$
$EPC_{LH} = 0.2 \times 207 = 41.4$ $\mu g/g$

$EPC_{WE1} = 50 \times 100 = 5{,}000$ $\mu g/\ell$
$EPC_{WE2} = 5{,}000$ $\mu g/\ell$ (to prevent tainting)
$EPC_{LE} = 0.2 \times 5{,}000 = 1{,}000$ $\mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

X
23A020
PYRIDINE

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)			1.5E4 (5)		35.7 (0.012)		67.7
Water, μg/l (ppm Wt)			2.3E5	1.0E4	207	5,000	
Land, μg/g (ppm Wt)			4.5E4	2.0E3	41.4	1.0E3	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

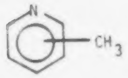
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)			35.7 (0.012)		
Water, μg/l (ppm Wt)			207	5,000	
Land, μg/g (ppm Wt)			41.4	1,000	

CATEGORY: 23A

WLN:

PICOLINES: C_6H_7N (Methylpyridines). 23A040
2-METHYLPYRIDINE: 23A041
3-METHYLPYRIDINE: 23A042
4-METHYLPYRIDINE: 23A043

STRUCTURE:



The pyridines have a strong, unpleasant odor.

PROPERTIES:

Molecular wt: 93.14; bp: 129-145; d: 0.95 to 0.97_4^{15};
pK_a: 5.68-5.96 (ref. 1); soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Pyridine, picolines, and lutidines are usually obtained by the degradation of coal. They display aromaticity in their substitution reactions. As bases they are less basic than aliphatic amines (ref. 4).

Pyridine and pyridine-ring compounds are photolytically active (ref. 2).

Threshold odor concentration for 2-methylpyridine is 0.023 ppm (ref. 10).

TOXIC PROPERTIES, HEALTH EFFECTS:

The picolines are irritating to the eyes and to the respiratory tract (ref. 11).

	LD_{50} (oral, rat) (ref. 7)	LD_{100} (inhalation, rat) (ref. 11)
2-picoline	790 mg/kg	15,400 ppm/1.5 hr
3-picoline	800 mg/kg	8,700 ppm/2.2 hr
4-picoline	800 mg/kg	8,000 ppm/2 hr

Certain pyridine compounds are reported to cause tainting of fish (ref. 9).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 790 = 3.56 \times 10^4\ \mu g/m^3$
Water, Health: $15 \times 3.56 \times 10^4 = 5.34 \times 10^5\ \mu g/\ell$
Land, Health: $0.2 \times 5.33 \times 10^5 = 1.07 \times 10^5\ \mu g/g$

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 790 = 84.5\ \mu g/m^3$
$EPC_{AH3} = 0.081 \times 790 = 64.0\ \mu g/m^3$
$EPC_{WH} = 15 \times 64 = 960\ \mu g/\ell$
$EPC_{WH2} = 0.4 \times 790 = 316\ \mu g/\ell$
$EPC_{LH} = 0.2 \times 316 = 63.2\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

23A040 PICOLINES

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			3.6E4		64		
Water, $\mu g/l$ (ppm Wt)			5.3E5		316		
Land, $\mu g/g$ (ppm Wt)			1.1E5		63		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			64		
Water, $\mu g/l$ (ppm Wt)			316		
Land, $\mu g/g$ (ppm Wt)			63		

CATEGORY: 23A

MONOSUBSTITUTED ALKYL PYRIDINES: 23A060

2-ETHYLPYRIDINE: A liquid. C_7H_9N 23A061

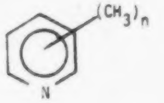
3-ETHYLPYRIDINE: A colorless to brownish liquid. C_7H_9N 23A062

4-ETHYLPYRIDINE: A liquid with an obnoxious odor. C_7H_9N 23A063

4-n-PROPYLPYRIDINE: A liquid. $C_8H_{11}N$ 23A064

WLN:

STRUCTURE:



PROPERTIES:	mol.wt.	mp.	bp.	d.	vap.d.	solubility in water
2-ethylpyridine:	107.16	-63.1	148.6	0.9502		soluble
3-ethylpyridine:	107.16	-76.9	165	0.9539		soluble
4-ethylpyridine:	107.16	-90.5	167.7	0.9417	3.70	soluble
4-n-propylpyridine:	121.18	-	184.6	0.9381		slightly

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Alkyl pyridines are used mainly as solvents or intermediates in chemical syntheses and in the manufacture of pharmaceuticals and resins (ref. 11).

TOXIC PROPERTIES, HEALTH EFFECTS:

4-Ethylpyridine is reported to exhibit toxic effects similar to pyridine (ref. 12).

Alkyl derivatives are absorbed from the gastrointestinal tract, intraperitoneal cavity, and lungs. The toxicity and irritant properties of the derivatives substituted at the 4 position tend to be greater than the corresponding derivatives substituted at the 2 position. This is reported for inhalation exposure as well as other routes of administration (ref. 11).

Chemical	LC_{100} (inhalation, rats)	
	ppm	time for 100% mortality, hr.
2-ethylpyridine	5,400	3.0
4-ethylpyridine	2,500	5.0
4-n-propylpyridine	1,000	6.0

The data given above indicates that the monosubstituted alkyl pyridines considered have toxicological characteristics similar to collidines: LC_{100} (inhalation, rat): 2,500 ppm; LD_{50} (oral, rat): 1,540 mg/kg; aquatic toxicity: TLm 96: 100 - 1,000 ppm (ref. 7).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 1{,}540 = 6.93 \times 10^4$ μg/m^3

Water, Health: $15 \times 6.93 \times 10^4 = 1.04 \times 10^6$ μg/l

Land, Health: $0.2 \times 1.04 \times 10^6 = 2.08 \times 10^5$ μg/g

Air, Ecology:

Water, Ecology: $100 \times 100 = 1.0 \times 10^4$ μg/l

Land, Ecology: $0.2 \times 1.0 \times 10^4 = 2{,}000$ μg/g

* ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 1{,}540 = 165$ μg/m^3

$EPC_{AH3} = 0.081 \times 1{,}540 = 125$ μg/m^3

$EPC_{WH1} = 15 \times 125 = 1{,}875$ μg/l

$EPC_{WH2} = 0.4 \times 1{,}540 = 616$ μg/l

$EPC_{LH} = 0.2 \times 616 = 123.2$ μg/g

$EPC_{WE1} = 50 \times 100 = 5{,}000$ μg/l

$EPC_{LE} = 0.2 \times 5{,}000 = 1{,}000$ μg/g

*Based on LD_{50} (oral, rat): 1,540 mg/kg for col[illegible]

MULTIMEDIA ENVIRONMENTAL GOALS

23A060
MONOSUBSTITUTED ALKYL PYRIDINES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent [†]		B. Ambient Level Goal* [†]		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			6.9E4		125		
Water, μg/l (ppm Wt)			1.0E6	1.0E4	616	5,000	
Land, μg/g (ppm Wt)			2.1E5	2.0E3	123.2	1,000	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration [†]		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			125		
Water, μg/l (ppm Wt)			616	5,000	
Land, μg/g (ppm Wt)			123.2	1,000	

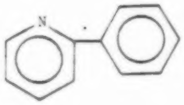
[†] Based on data for collidines.

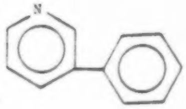
CATEGORY: 23A

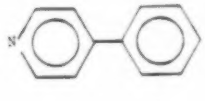
WLN:

PHENYLPYRIDINES:: $C_{11}H_9N$ 23A080
2-PHENYLPYRIDINE: (α-pyridylbenzene). A liquid. 23A081
3-PHENYLPYRIDINE: (β-pyridylbenzene). An oily liquid. 23A082
4-PHENYLPYRIDINE: (γ-pyridylbenzene). A solid. 23A083

STRUCTURE:







PROPERTIES:	mol.wt.	mp.	bp.	d.	solubility in water
2-phenylpyridine	155.2		$270\text{-}2^{760}$	1.0833^{25}	slightly
3-phenylpyridine	155.2		273^{760}		slightly
4-phenylpyridine	155.2	77-8	$280\text{-}2^{762}$		soluble in hot water

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Radical arylation of pyridine gives a mixture of all 3 isomers, in which the 2-isomer is usually the main component (ref. 13).

Phenyl addition to pyridine will result in a less water soluble compound.

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for phenylpyridines are not available at this time. However, toxicological characteristics of phenylpyridines are likely to be similar to monosubsubstituted alkyl pyridines and collidines.

LD_{50} (oral, rat): 1,540 mg/kg for collidines.
TLm 96: 100 to 1,000 for collidines.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

* **MINIMUM ACUTE TOXICITY CONCENTRATIONS**:

Air, Health: $45 \times 1,540 = 6.93 \times 10^4$ µg/m^3
Water, Health: $15 \times 6.93 \times 10^4 = 1.04 \times 10^6$ µg/l
Land, Health: $0.2 \times 1.04 \times 10^6 = 2.08 \times 10^5$ µg/g

Air, Ecology:
Water, Ecology: $100 \times 100 = 1.0 \times 10^4$ µg/l
Land, Ecology: $0.2 \times 1.0 \times 10^4 = 2,000$ µg/g

* **ESTIMATED PERMISSIBLE CONCENTRATIONS**:

$EPC_{AH2} = 0.107 \times 1,540 = 165$ µg/m^3
$EPC_{AH3} = 0.081 \times 1,540 = 125$ µg/m^3
$EPC_{WH1} = 15 \times 125 = 1,875$ µg/l
$EPC_{WH2} = 0.4 \times 1,540 = 616$ µg/l
$EPC_{LH} = 0.2 \times 616 = 123.2$ µg/g

$EPC_{WE1} = 50 \times 100 = 5,000$ µg/l
$EPC_{LE} = 0.2 \times 5,000 = 1,000$ µg/g

*Based on data available for collidines.

MULTIMEDIA ENVIRONMENTAL GOALS

23A080
PHENYLPYRIDINES

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent †		B. Ambient Level Goal* †		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			6.9E4		125		
Water, $\mu g/l$ (ppm Wt)			1.0E6	1.0E4	616	5,000	
Land, $\mu g/g$ (ppm Wt)			2.1E5	2.0E3	123	1,000	

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration †		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			125		
Water, $\mu g/l$ (ppm Wt)			616	5,000	
Land, $\mu g/g$ (ppm Wt)			123	1,000	

† Based on data for collidines.

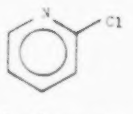
CATEGORY: 23A

CHLOROPYRIDINES: C_5H_4ClN 23A100
2-CHLOROPYRIDINE: A liquid 23A101
3-CHLOROPYRIDINE: A liquid 23A102
4-CHLOROPYRIDINE: A liquid 23A103

WLN:

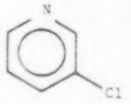
STRUCTURE:

T6NJ BG /



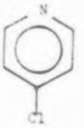
2-chloropyridine

T6NJ CG /



3-chloropyridine

T6NJ DG /



4-chloropyridine

PROPERTIES:

	mol.wt.	bp.	d.	vap.d.	vap.press	solubility in water
2-chloropyridine:	113.55	170^{760}	1.205^{15}	3.93	1mm at 13.3	slight
3-chloropyridine:	113.55	148^{744}				slight
4-chloropyridine:	113.55	147^{744}				slight

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

4-Chloropyridine has been reported in samples taken from river water and finished drinking water (ref. 14).

Chloropyridines will react with ammonia at 180-200° to form aminopyridines.

3-Chloropyridine is used in the manufacture of pharmaceuticals, germicides, and pesticides. The compound is also formed during chlorination, when pyridine is present in water (ref. 10).

TOXIC PROPERTIES, HEALTH EFFECTS:

Aminopyridines, which can be formed from chloropyridine, can be very toxic, especially the 2-aminopyridine isomer. Three separate cases of human intoxication from exposure to 2-aminopyridine have been reported, one case resulting in death (ref. 11).

Chemical	LD_{50} (intraperitoneal, mouse) (mg/kg)	LD_{50} (intraperitoneal, rat) (mg/kg)	LC_{Lo} (inhalation, rat)
2-chloropyridine	130		250ppm/7hours
3-chloropyridine	235		
4-chloropyridine		275	

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

*MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 130 = 5{,}850\ \mu g/m^3$

Water, Health: $15 \times 5{,}850 = 8.78 \times 10^4\ \mu g/l$

Land, Health: $0.2 \times 8.78 \times 10^4 = 1.76 \times 10^4\ \mu g/g$

Air, Ecology:

Water, Ecology:

Land, Ecology:

*ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 130 = 13.9\ \mu g/m^3$

$EPC_{AH3} = 0.081 \times 130 = 10.5\ \mu g/m^3$

$EPC_{WH1} = 15 \times 10.5 = 157.5\ \mu g/l$

$EPC_{WH2} = 0.4 \times 130 = 52.0\ \mu g/l$

$EPC_{LH} = 0.2 \times 52 = 10.4\ \mu g/g$

*Based on LD_{50} (intraperitoneal, mouse) for 2-chloropyridine.

MULTIMEDIA ENVIRONMENTAL GOALS

X
23A100
CHLOROPYRIDINES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			5.9E3		10.5		
Water, $\mu g/l$ (ppm Wt)			8.8E4		52		
Land, $\mu g/g$ (ppm Wt)			1.8E4		10.4		

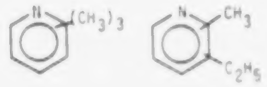
*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			10.5		
Water, $\mu g/l$ (ppm Wt)			52		
Land, $\mu g/g$ (ppm Wt)			10.4		

CATEGORY: 23A

WLN: T6NJ B E2

STRUCTURE:



COLLIDINES: $C_8H_{11}N$ (trimethylpyridines, ethyl methyl pyridines). 23A120
5-ETHYL-2-METHYLPYRIDINE: (3-ethyl-6-methylpyridine). 23A121
2,4,6-COLLIDINE: 23A122

PROPERTIES:

Molecular wt: 121.18; bp: 165-198; d: 0.9130-0.9352; pk_a: 7.1-7.45 (ref. 1); sparingly soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Collidines are found in low temperature tar. In general, they exhibit characteristics of aromatic compounds. As bases they are stronger than pyridine.

Pyridine and its derivatives are photolytically active (ref. 2).

Threshold odor for 2-methyl-5-ethyl pyridine is 0.008 ppm (ref. 10). It has been reported in samples taken from finished drinking water (ref. 14).

The compound 2,4,6-collidine is produced in coal carbonization processes (ref. 3).

TOXIC PROPERTIES, HEALTH EFFECTS:

The simple alkyl derivatives of pyridine act as local irritants (ref. 11). 2-Methyl-5-ethyl-pyridine is listed as a corrosive liquid (ref. 7).

LD_{50} (oral, rat): 1,540 mg/kg for 5-ethyl-2-methylpyridine.

Aquatic toxicity: The 96-hr TLm for 2-ethyl-5-methyl pyridine is reported as 100 to 1,000 ppm (ref. 7). Certain pyridine compounds cause tainting of fish flesh (ref. 9).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 1,540 = 6.93 \times 10^4\ \mu g/m^3$
Water, Health: $15 \times 6.93 \times 10^4 = 1.04 \times 10^6\ \mu g/\ell$
Land, Health: $0.2 \times 1.04 \times 10^6 = 2.08 \times 10^5\ \mu g/g$

Air, Ecology:
Water, Ecology: $100 \times 100 = 1.0 \times 10^4\ \mu g/\ell$
Land, Ecology: $0.2 \times 1.0 \times 10^4 = 2,000\ \mu g/g$

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 1,540 = 165\ \mu g/m^3$
$EPC_{AH3} = 0.081 \times 1,540 = 125\ \mu g/m^3$
$EPC_{WH1} = 15 \times 125 = 1,875\ \mu g/\ell$
$EPC_{WH2} = 0.4 \times 1,540 = 616\ \mu g/\ell$
$EPC_{LH} = 0.2 \times 616 = 123.2\ \mu g/g$

$EPC_{WE1} = 50 \times 100 = 5,000\ \mu g/\ell$
$EPC_{LE} = 0.2 \times 5,000 = 1,000\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

23A120
COLLIDINES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			6.9E4		125		
Water, $\mu g/l$ (ppm Wt)			1.0E6	1.0E4	616	5,000	
Land, $\mu g/g$ (ppm Wt)			2.1E5	2.0E3	123	1,000	

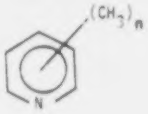
*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			125		
Water, $\mu g/l$ (ppm Wt)			616	5,000	
Land, $\mu g/g$ (ppm Wt)			123	1,000	

CATEGORY: 23A

DISUBSTITUTED, POLYSUBSTITUTED ALKYL PYRIDINES: 23A140

2,3-DIMETHYLPYRIDINE: $(CH_3)_2C_5H_3N$ · (2,3-lutidine) A liquid. 23A141
2,4-DIMETHYLPYRIDINE: $(CH_3)_2C_5H_3N$ · (2,4-lutidine) A liquid. 23A142
2,5-DIMETHYLPYRIDINE: $(CH_3)_2C_5H_3N$ · (2,5-lutidine) A liquid. 23A143
2,6-DIMETHYLPYRIDINE: $(CH_3)_2C_5H_3N$ · (2,6-lutidine) A liquid. 23A144
3,4-DIMETHYLPYRIDINE: $(CH_3)_2C_5H_3N$ · (3,4-lutidine) A liquid. 23A145
2,3,4,6-TETRAMETHYLPYRIDINE: $(CH_3)_4C_5H_1N$. (β-parvalone). A liquid. 23A146



PROPERTIES:

	mol.wt.	mp.	bp.	d.	solubility in water
2,3-dimethylpyridine	107.15		163.4	0.9319	soluble
2,4-dimethylpyridine	107.15		159-9.5	0.9309	soluble
2,5-dimethylpyridine	107.15	-16	156.8-.9	0.9297	slightly
2,6-dimethylpyridine	107.15	-6.1	145.7	0.9226	soluble
3,4-dimethylpyridine	107.15		163.5	0.9281	slightly
2,3,4,6-tetramethylpyridine	135.21	230 (decomposes)		-	slightly

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Disubstituted and polysubstituted alkyl pyridines, including lutidines, are used mainly as special solvents or intermediates in chemical syntheses and in the manufacture of pharmaceuticals and resins (ref. 11). Lutidines were first isolated from bone oil, and are found principally in coal tar, and in general, exhibit properties characterisitc of aromatic compounds (ref. 11).

TOXIC PROPERTIES, HEALTH EFFECTS:

Alkyl derivatives of pyridine are absorbed from the gastrointestinal tract, intraperitoneal cavity, and lungs. In order of decreasing toxicity, dimethylpyridines follow 2-aminopyridine, vinyl pyridine, amyl pyridines, and collidine and are more toxic than pyridine (ref. 11). The toxicity and irritant properties of the pyridine derivatives substituted at the 4 position tend to be greater than the corresponding derivatives substituted at the 2 position. This is true for inhalation exposures as well as other routes of administration (ref. 11)

Data for the di- and polysubstituted alkyl pyridines are given below.

Chemical	LD_{50}(oral,rat) (mg/kg)	LC_{100}(inhalation,rat) ppm
2,3-dimethylpyridine	400 (ref. 11)	-
2,4-dimethylpyridine	-	4,300/2 hr (ref. 11)
2,5-dimethylpyridine	800 (ref. 7)	-
2,6-dimethylpyridine	-	7,500/1.2 hr (ref. 11)
3,4-dimethylpyridine	710 (ref. 7)	-

***MINIMUM ACUTE TOXICITY CONCENTRATIONS**:

Air, Health:	$45 \times 400 = 1.8 \times 10^4$ μg/m^3	Air, Ecology:
Water, Health:	$15 \times 1.8 \times 10^4 = 2.7 \times 10^5$ μg/l	Water, Ecology:
Land, Health:	$0.2 \times 2.7 \times 10^5 = 5.4 \times 10^4$ μg/g	Land, Ecology:

***ESTIMATED PERMISSIBLE CONCENTRATIONS**:

$EPC_{AH2} = 0.107 \times 400 = 42.8$ μg/m^3

$EPC_{AH3} = 0.081 \times 400 = 32.4$ μg/m^3

$EPC_{WH1} = 15 \times 32.4 = 486$ μg/l

$EPC_{WH2} = 0.4 \times 400 = 160$ μg/l

$EPC_{LH} = 0.2 \times 160 = 32$ μg/g

*Based on LD_{50} (oral, rat) for 2,3-dimethylp

MULTIMEDIA ENVIRONMENTAL GOALS

X

23A140

DISUBSTITUTED, POLYSUBSTITUTED ALKYL PYRIDINES

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.8E4		32.4		
Water, $\mu g/l$ (ppm Wt)			2.7E5		160		
Land, $\mu g/g$ (ppm Wt)			5.4E4		32		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			32.4		
Water, $\mu g/l$ (ppm Wt)			160		
Land, $\mu g/g$ (ppm Wt)			32		

371<

REFERENCES: CATEGORY 23A

Heterocyclic Nitrogen Compounds - Pyridine and Substituted Pyridines

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CATEGORY 23

HETEROCYCLIC NITROGEN COMPOUNDS

SUBCATEGORY: 23B - Fused Six-Membered Ring Heterocycles

Summary of Subcategory

Total number of compounds in subcategory	22
number of parent compounds with subspecies	2
number of subspecies	9
Number of parent compounds with no MEG values	2
Number of parent compounds with natural background levels only	1
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	4

Consent Decree compounds included in subcategory: 0

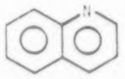
CATEGORY: 23B

WLN: T66 BNJ
T66 CNJ

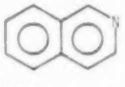
QUINOLINES: 23B020
QUINOLINE: C_9H_7N (1-benzazine, chinoline, benzo(b)pyridine).23B021
ISOQUINOLINE: (leucoline, benzo(c)pyridine). 23B022
Liquids with strong odors.

STRUCTURE:

Quinoline



Isoquinoline



PROPERTIES:

Quinoline: Molecular wt: 129.16; mp: -15; bp: 237.7; d: 1.09^{25}_{4}; vap. press: 1 mm at 59.7° C; soluble in hot water.

Isoquinoline: Molecular wt: 129.1; mp: 26.48; d: 1.091^{30}_{4}; slightly soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Quinoline and isoquinoline are isolated in small amounts from coal tar. They are less basic than aliphatic amines. Compounds containing the pyridine ring are photolytically active (ref. 1). Odor threshold for quinoline is 0.7 ppm (ref. 2). Quinoline and isoquinoline have both been identified in the ambient urban air in concentrations up to 69 ng/1000 m^3 and 180 ng/1000 m^3, respectively (ref. 3).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicity information for quinoline is very sparse. It is a mild irritant.
LD_{50} (oral, rat): 460 mg/kg for quinoline.
LD_{50} (oral, rat): 350 mg/kg for isoquinoline.
Concentrations of 0.5 to 1.0 mg/ℓ in water may cause tainting of fish flesh (ref. 4,5).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: 45 x 350 = 1.58×10^4 μg/m^3	Air, Ecology:
Water, Health: 15 x 1.58×10^4 = 2.36×10^5 μg/ℓ	Water, Ecology:
Land, Health: 0.2 x 2.36×10^5 = 4.72×10^4 μg/g	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

EPC_{AH2} = 0.107 x 350 = 37.5 μg/m^3
EPC_{AH3} = 0.081 x 350 = 28.4 μg/m^3
EPC_{WH1} = 15 x 28.4 = 426 μg/ℓ
EPC_{WH2} = 0.4 x 350 = 140 μg/ℓ
EPC_{LH} = 0.2 x 140 = 28 μg/g

EPC_{WE1} = 500 (to prevent tainting) μg/ℓ

EPC_{LE} = 0.2 x 500 = 100 μg/g

23B020
QUINOLINES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			1.6E4		28.4		
Water, μg/l (ppm Wt)			2.4E5		140	500	
Land, μg/g (ppm Wt)			4.7E4		28	100	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			28.4		
Water, μg/l (ppm Wt)			140	500	
Land, μg/g (ppm Wt)			28	100	

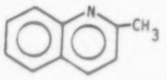
CATEGORY: 23B

WLN: T66 BNJ C

2-METHYLQUINOLINE: $C_{10}H_9N$ (quinaldine). 23B040

Colorless, oily liquid with quinoline-like odor.

STRUCTURE:



PROPERTIES:

Molecular wt: 143.19; bp: 246-247; d: 1.06;
insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

2-methylquinoline occurs in small amounts in coal tar. In general, it exhibits properties of aromatic compounds. Compounds containing the pyridine ring are photolytically active (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

2-methylquinoline is a respiratory tract irritant (ref. 6).

LD_{50} (oral, rat): 1,230 mg/kg.

Certain quinoline compounds are reported to cause tainting of fish (ref. 4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 1{,}230 = 5.54 \times 10^4$ μg/m^3
Water, Health: $15 \times 5.54 \times 10^4 = 8.31 \times 10^5$ μg/ℓ
Land, Health: $0.2 \times 8.31 \times 10^5 = 1.66 \times 10^5$ μg/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 1{,}230 = 132$ μg/m^3
$EPC_{AH3} = 0.081 \times 1{,}230 = 100$ μg/m^3
$EPC_{WH1} = 15 \times 100 = 1{,}500$ μg/ℓ
$EPC_{WH2} = 0.4 \times 1{,}230 = 492$ μg/ℓ
$EPC_{LH} = 0.2 \times 492 = 98$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

23B040
2-METHYLQUINOLINE

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m³ (ppm Vol)			5.5E4		100		
Water, μg/l (ppm Wt)			8.3E5		492		
Land, μg/g (ppm Wt)			1.7E5		98		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

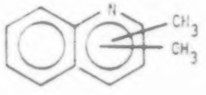
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m³ (ppm Vol)			100		
Water, μg/l (ppm Wt)			492		
Land, μg/g (ppm Wt)			98		

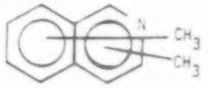
CATEGORY: 23B

DIMETHYLQUINOLINES AND DIMETHYLISOQUINOLINES: $C_{11}H_{11}N$ 23B060
2,3-DIMETHYLQUINOLINE: (3-methylquinaldine). A solid. 23B061
2,6-DIMETHYLQUINOLINE: (6-methylquinaldine). A solid. 23B062
2,8-DIMETHYLQUINOLINE: (o-toluquinaldine). A solid. 23B063
3,4-DIMETHYLQUINOLINE: (3-methyllepidine). A solid. 23B064
6,8-DIMETHYLQUINOLINE: (β-cytisolidine). A liquid. 23B065
1,3-DIMETHYLISOQUINOLINE: A solid or liquid. 23B066
1,5-DIMETHYLISOQUINOLINE: A solid. 23B067

WLN:

STRUCTURE:





PROPERTIES:

	mol.wt.	mp.	bp.	d.	solubility in water
2,3-dimethylquinoline:	157.22	68-9	261^{729}	1.1013	insoluble
2,6-dimethylquinoline:	157.22	60	266-7		slightly in hot water
2,8-dimethylquinoline:	157.22	27	255.3^{760}	1.0394_4^{20}	slight
3,4-dimethylquinoline:	157.22	73-4	290^{737}		insoluble
6,8-dimethylquinoline:	157.22		$268\text{-}9^{760}$	1.0665	slight
1,3-dimethylisoquinoline:	157.22	30	262		
1,5-dimethylisoquinoline:	157.22	97-8			

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Substituted quinolines are likely to be associated with particulate polycyclic aromatic hydrocarbons. Dimethylquinoline and dimethylisoquinoline have both been identified in ambient urban air (ref. 3).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for dimethylquinolines and dimethylisoquinolines are not available at this time. However, toxicological characteristics of these compounds are likely to be most similar to those of methylquinoline.

Substance	LD_{50}(oral, rat)(mg/kg)	Substance	LD_{50}(oral, rat)(mg/kg)
pyridine	891	quinoline	460
methylpyridine	800	methylquinoline	1,230
dimethylpyridine	400-800		
trimethylpyridine	1,540		

The available data indicate that methylation of pyridine and quinoline usually does not increase the toxicity of these compounds.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m³ (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

***MINIMUM ACUTE TOXICITY CONCENTRATIONS**:

Air, Health: $45 \times 1{,}230 = 5.54 \times 10^4$ μg/m³ Air, Ecology:

Water, Health: $15 \times 5.54 \times 10^4 = 8.31 \times 10^5$ μg/l Water, Ecology:

Land, Health: $0.2 \times 8.31 \times 10^5 = 1.66 \times 10^5$ μg/g Land, Ecology:

***ESTIMATED PERMISSIBLE CONCENTRATIONS**:

$EPC_{AH2} = 0.107 \times 1{,}230 = 132$ μg/m³

$EPC_{AH3} = 0.081 \times 1{,}230 = 100$ μg/m³

$EPC_{WH1} = 15 \times 100 = 1{,}500$ μg/l

$EPC_{WH2} = 0.4 \times 1{,}230 = 492$ μg/l

$EPC_{LH} = 0.2 \times 492 = 98$ μg/g

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*Based on methylquinoline LD_{50} (oral, rat): 1,230 mg/kg.

MULTIMEDIA ENVIRONMENTAL GOALS

23B060
DIMETHYLQUINOLINES

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent †		B. Ambient Level Goal* †		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			5.54E4		100		
Water, $\mu g/l$ (ppm Wt)			8.31E5		492		
Land, $\mu g/g$ (ppm Wt)			1.7E5		98		

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects †	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			100		
Water, $\mu g/l$ (ppm Wt)			492		
Land, $\mu g/g$ (ppm Wt)			98		

†Based on data for methylquinoline.

380<

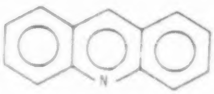
CATEGORY: 23B

WLN: T C666 BNJ

ACRIDINE: $C_{13}H_9N$ (10-azaanthracene, benzo(b)quinoline, dibenzo(b,e)pyridine). 23B080

Small colorless crystals, dilute solutions exhibit violet fluorescence.

STRUCTURE:



PROPERTIES:

Molecular wt: 179.21; mp: 111; sublimes; bp: 345-346; pK_a: 5.6 (ref. 7) d: 1.005^{20}; vap. press.: 1 mm at 129.4°; slightly soluble in hot water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Acridines may be found in coal tar and pitch. They are associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 8). The concentration of acridine in urban atmosphere is reported as 0.67 $\mu g/1{,}500\ m^3$ (ref. 9). This is equivalent to 0.00045 $\mu g/m^3$.

The acridines are classified as weak bases.

TOXIC PROPERTIES, HEALTH EFFECTS:

Acridine is irritating to skin and to mucous membranes (ref. 7). Acridine may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man (7, 10). There is no evidence to indicate that acridine alone is carcinogenic to man or to animals.

LD_{50} (oral, rat): 2,000 mg/kg.

Acridine is reported to be toxic to fish at 5 mg/ℓ (ref. 2).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV (coal tar pitch volatiles): 0.2 mg/m^3. [The specification includes naphthalene, anthracene, acridine, phenanthrene, and fluorene, collectively. The purpose of the TLV is to minimize concentrations of higher-weight polycyclic hydrocarbons which are carcinogenic (ref. 11).]

A candidate for the list for EPA Toxic Pollutant Effluent Standards (ref. 12).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 2{,}000 = 9.0 \times 10^4\ \mu g/m^3$
Water, Health: $15 \times 9.0 \times 10^4 = 1.35 \times 10^6\ \mu g/\ell$
Land, Health: $0.2 \times 1.35 \times 10^6 = 2.70 \times 10^5\ \mu g/g$

Air, Ecology:
Water, Ecology: $100 \times 5 = 500\ \mu g/\ell$
Land, Ecology: $0.2 \times 500 = 100\ \mu g/g$

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 2{,}000 = 214\ \mu g/m^3$
$EPC_{AH3} = 0.081 \times 2{,}000 = 162\ \mu g/m^3$
$EPC_{WH1} = 15 \times 162 = 2{,}430\ \mu g/\ell$
$EPC_{WH2} = 0.4 \times 2{,}000 = 800\ \mu g/\ell$
$EPC_{LH} = 0.2 \times 800 = 160\ \mu g/g$

$EPC_{WE1} = 50 \times 5 = 250\ \mu g/\ell$

$EPC_{LE} = 0.2 \times 250 = 50\ \mu g/g$

23B080
ACRIDINE

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			9.0E4		162		0.00045†
Water, μg/l (ppm Wt)			1.4E6	5.0E2	800	250	
Land, μg/g (ppm Wt)			2.7E5	1.0E2	160	50	

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			162		
Water, μg/l (ppm Wt)			800	250	
Land, μg/g (ppm Wt)			160	50	

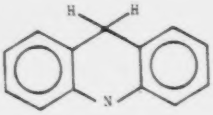
†Reported for urban atmosphere. No rural concentration is reported.

CATEGORY: 23B

DIHYDROACRIDINE: $C_{13}H_{11}N$ (acridan, carbazine). 23B100
A solid.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 181.24; mp:169-71; decomposes at 300°; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Dihydroacridine is likely to be associated with particulate polycyclic aromatic hydrocarbons.

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{50} (subcutaneous, mouse): 3,630 μg/kg (ref. 13).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	45 x 3.63 = 163.4 μg/m^3	Air, Ecology:	
Water, Health:	15 x 163.4 = 2,451 μg/l	Water, Ecology:	
Land, Health:	0.2 x 2,451 = 490.2 μg/g	Land, Ecology:	

ESTIMATED PERMISSIBLE CONCENTRATIONS:

EPC_{AH2} = 0.107 x 3.63 = 0.39 μg/m^3

EPC_{AH3} = 0.081 x 3.63 = 0.29 μg/m^3

EPC_{WH1} = 15 x 0.29 = 4.35 μg/l

EPC_{WH2} = 0.4 x 3.63 = 1.45 μg/l

EPC_{LH} = 0.2 x 1.45 = 0.29 μg/g

383<

MULTIMEDIA ENVIRONMENTAL GOALS

X
23B100
DIHYDROACRIDINE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.6E2		0.3		
Water, $\mu g/l$ (ppm Wt)			2.5E3		1.5		
Land, $\mu g/g$ (ppm Wt)			4.9E2		0.3		

*To be multiplied by dilution factor

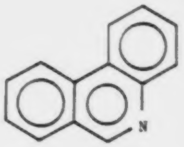
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			0.3		
Water, $\mu g/l$ (ppm Wt)			1.5		
Land, $\mu g/g$ (ppm Wt)			0.3		

CATEGORY: 23B

PHENANTHRIDINE: $C_{13}H_9N$ (3,4-benzoquinoline, 9-azaphenanthrene, benzo(c)quinoline). 23B120
A solid.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 179.22; mp: 106-7; bp: 349^{769}; slightly soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Phenanthridine can be produced from quinoline in the presence of furan and lithium amalgam (ref. 15). It has been identified in the ambient air of New York City at a concentration of 22 ng/1000 m^3 (ref. 3).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for phenanthridine are not available at this time. However, toxicological characteristics of phenanthridine are likely to be similar to those of acridine because of the chemical structure similarity.

Certain nitrogen containing heterocyclics are known to induce tumor formation in experimental animals (ref. 14).

Certain quinoline compounds are reported to cause tainting of fish (ref. 4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg.m^3 (for particulate polycylic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

*MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$45 \times 2{,}000 = 9.0 \times 10^4$ µg/m^3	Air, Ecology:
Water, Health:	$15 \times 9.0 \times 10^4 = 1.35 \times 10^6$ µg/l	Water, Ecology:
Land, Health:	$0.2 \times 1.35 \times 10^6 = 2.70 \times 10^5$ µg/g	Land, Ecology:

*ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 0.107 \times 2{,}000 = 214$ µg/m^3

$EPC_{AH2} = 0.081 \times 2{,}000 = 162$ µg/m^3

$EPC_{WH1} = 15 \times 162 = 2{,}430$ µg/l

$EPC_{WH2} = 0.4 \times 2{,}000 = 800$ µg/l

$EPC_{LH} = 0.2 \times 800 = 160$ µg/g

*Based on LD_{50} (oral, rat): 2,000 mg/kg for acridine

MULTIMEDIA ENVIRONMENTAL GOALS

23B120
PHENANTHRIDINE

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent †		B. Ambient Level Goal* †		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			9.0E4		162		
Water, $\mu g/l$ (ppm Wt)			1.4E6		800		
Land, $\mu g/g$ (ppm Wt)			2.7E5		160		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration †		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			162		
Water, $\mu g/l$ (ppm Wt)			800		
Land, $\mu g/g$ (ppm Wt)			160		

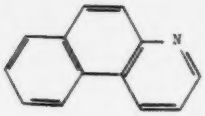
†Based on data for acridine.

CATEGORY: 23B

BENZO(f)QUINOLINE: $C_{13}H_9N$ (5,6-benzoquinoline, β-naphthoquinoline, naphthopyridine). A solid. 23B140

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 179.22; mp:94; bp:350^{721}; slightly soluble in hot water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzo(f)quinoline is used as a reagent for the determination of cadmium, which is precipitated as $(C_{13}H_9N)_2H_2$ (CdI_4) from dilute nitric or sulfuric acid solution in the presence of potassium iodide (ref. 16).

Benzo(f)quinoline concentration in the average U.S. urban atmosphere is reported as 0.2 μg/1,000 m^3 air (refs. 14,17). It is associated with particulate polycyclic aromatic hydrocarbons.

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for benzo(f)quinoline are not available at this time. However, toxicological characteristics of benzo(f)quinoline are likely to be similar to those of acridine because of the chemical structure similarity.

Certain nitrogen containing heterocyclics are known to induce tumor formation in experimental animals (ref. 14).

Certain quinoline compounds are reported to cause tainting of fish (ref. 4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarcons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

*MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Heatlh:	$45 \times 2{,}000 = 9.0 \times 10^4$ $\mu g/m^3$	Air, Ecology:
Water, Health:	$15 \times 9.0 \times 10^4 = 1.35 \times 10^6$ $\mu g/l$	Water, Ecology:
Land, Health:	$0.2 \times 1.35 \times 10^6 = 2.70 \times 10^5$ $\mu g/g$	Land, Ecology:

*ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 0.107 \times 2{,}000 = 214$ $\mu g/m^3$

$EPC_{AH2} = 0.081 \times 2{,}000 = 162$ $\mu g/m^3$

$EPC_{WH1} = 15 \times 162 = 2{,}430$ $\mu g/l$

$EPC_{WH2} = 0.4 \times 2{,}000 = 800$ $\mu g/l$

$EPC_{LH} = 0.2 \times 800 = 160$ $\mu g/g$

*Based on LD_{50} (oral, rat): 2,000 mg/kg for acridine.

MULTIMEDIA ENVIRONMENTAL GOALS

23B140 BENZO(f)QUINOLINE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent ‡		B. Ambient Level Goal* ‡		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			9.0E4		162		0.2×10^{-3} †
Water, $\mu g/l$ (ppm Wt)			1.35E6		800		
Land, $\mu g/g$ (ppm Wt)			2.7E5		160		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated ‡ Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			162		
Water, $\mu g/l$ (ppm Wt)			800		
Land, $\mu g/g$ (ppm Wt)			160		

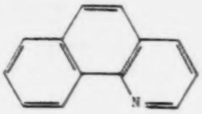
† Urban Atmosphere Concentration. Rural Concentration Is Not Available.

‡ Based on data for acridine.

CATEGORY: 238
BENZO(h)QUINOLINE: $C_{13}H_9N$ (7,8-benzoquinoline, α-naphthoquinoline). 238160
A solid.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 179.22; mp: 52; bp: 338^{719}; slightly soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzo(h)quinoline concentration in the average U.S. urban atmosphere is reported as 0.3 μg/1,000 m^3 air (refs. 17, 14). It is associated with particulate polycyclic aromatic hydrocarbons.

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for benzo(h)quinoline are not available at this time. However, toxicological characteristics of benzo(h)quinoline are likely to be similar to those of acridine because of the chemical structure similarity.

Certain nitrogen containing heterocyclics are known to induce tumor formation in experimental animals (ref. 14).

Certain quinoline compounds are reported to cause tainting of fish (ref. 4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycylic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

*MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$45 \times 2{,}000 = 9.0 \times 10^4$ μg/m3	Air, Ecology:
Water, Health:	$15 \times 9.0 \times 10^4 = 1.35 \times 10^6$ μg/l	Water, Ecology:
Land, Health:	$0.2 \times 1.35 \times 10^6 = 2.70 \times 10^5$ μg/g	Land, Ecology:

*ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH1} = 0.107 \times 2{,}000 = 214$ μg/m^3

$EPC_{AH2} = 0.081 \times 2{,}000 = 162$ μg/m^3

$EPC_{WH1} = 15 \times 162 = 2{,}430$ μg/l

$EPC_{WH2} = 0.4 \times 2{,}000 = 800$ μg/l

$EPC_{LH} = 0.2 \times 800 = 160$ μg/g

*Based on LD_{50} (oral, rat): 2,000 mg/kg for [illegible]

MULTIMEDIA ENVIRONMENTAL GOALS

23B160
BENZO(h)QUINOLINE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent †		B. Ambient Level Goal*†		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			9.0E4		162		3×10^{-4}
Water, $\mu g/l$ (ppm Wt)			1.4E6		800		
Land, $\mu g/g$ (ppm Wt)			2.7E5		160		

*To be multiplied by dilution factor

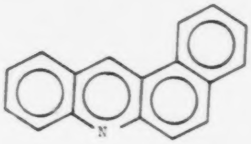
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated † Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			162		
Water, $\mu g/l$ (ppm Wt)			800		
Land, $\mu g/g$ (ppm Wt)			160		

† Based on data for acridine.

CATEGORY: 23B .
BENZ(a)ACRIDINE: $C_{17}H_{11}N$ (1,2-benzacridine). 23B180
A solid.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 229.29; pKa:3.95; solubility in water may be enhanced by the presence of acids as impurities in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Acridines may be found in coal tar and pitch. They are associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 8). The concentration of benz(a)acridine in average U.S. urban air is reported as 0.2 μg/1,000 m^3 (refs. 17, 14).

The acridines are classified as weak bases.

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for benz(a)acridine are not available at this time.

Certain nitrogen-containing heterocyclics are known to induce tumor formation in experimental animals (ref. 14).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0 2 mg/m^3 (for particulate polycyclic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

23B180
BENZ(a)ACRIDINE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							2×10^{-4}
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

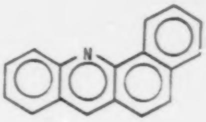
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

CATEGORY: 23B

WLN: T D6 B666 CNJ

BENZ(c)ACRIDINE: $C_{17}H_{11}N$ (α-chrysidine; α-naphthacridine; 3,4-benzacridine). 23B200
Benz(c)acridine crystallizes in the form of needles from aqueous ethanol; solutions show green fluorescence.

STRUCTURE:



PROPERTIES:

Molecular wt: 229.29; mp: 108; pK_a: 3.24 (ref. 14); solubility in water may be enhanced by the presence of acids as impurities in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Acridines may be found in coal tar and pitch. They are associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 8). The concentration of benz(c) acridine in air polluted with coal tar pitch is reported as 0.12 μg/1,000 m^3; and the average urban atmospheric concentration in the U.S. is reported as 0.6 μg/1,000 m^3 (ref. 10).

The acridines are classified as weak bases.

TOXIC PROPERTIES, HEALTH EFFECTS:

Benz(c)acridine may be present in soot, coal tar, and pitch which are known to be carcinogenic to man (refs. 7, 10). Although it is reported to cause tumors in mice, benz(c)acridine is not considered to be a highly active carcinogen. The EPA/NIOSH ordering number is 3121. The lowest dose to induce a carcinogenic response is reported as 468 mg/kg (ref. 13). The adjusted ordering number is 6.66.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 [for particulate polycyclic aromatic hydrocarbons (PPAH). This TLV recognizes the carcinogenic potential of PPAH collectively].

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/6.66 = 1.05 \times 10^4$ μg/m^3
Water, Health: $15 \times 1.05 \times 10^4 = 1.58 \times 10^5$ μg/ℓ
Land, Health: $0.2 \times 1.58 \times 10^5 = 3.16 \times 10^4$ μg/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 6.66) = 25.0$ μg/m^3
$EPC_{WC} = 15 \times 25 = 375$ μg/ℓ
$EPC_{LC} = 0.2 \times 375 = 75$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

23B200
BENZ(c)ACRIDINE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.1E4		25		0.0006†
Water, $\mu g/l$ (ppm Wt)			1.6E5		375		
Land, $\mu g/g$ (ppm Wt)			3.2E4		75		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					25
Water, $\mu g/l$ (ppm Wt)					375
Land, $\mu g/g$ (ppm Wt)					75

† Average for urban atmosphere. No rural concentration is reported.

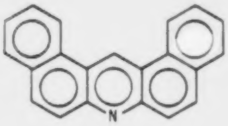
CATEGORY: 23B

WLN: T E6 D6 B666 NNJ

DIBENZ(a,j)ACRIDINE: $C_{21}H_{13}N$ (1,2:7,8-dibenzacridine). 23B220

Dibenz(a,j)acridine crystallizes as yellow needles. Sulfuric acid solutions of the compound exhibit greenish fluorescence.

STRUCTURE:



PROPERTIES:

Molecular wt: 279.35; mp: 216; solubility in water may be enhanced by the presence of acid impurities in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Acridines may be found in coal tar and pitch. They are associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 8).

The average atmospheric urban concentration of dibenz(a,j)acridine in the United States is reported as 0.04 ug/1,000 m^3 (ref. 14).

The acridines are classified as weak bases.

TOXIC PROPERTIES, HEALTH EFFECTS:

Dibenz(a,j)acridine may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man (refs. 7 , 10). Dibenz(a,j)acridine is reported to induce tumors in mice. The EPA/NIOSH ordering number if 3122. The lowest dose to induce an oncogenic response is 11 mg/kg (ref. 13). The adjusted ordering number is 284.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 [for particulate polycyclic aromatic hydrocarbons (PPAH). This TLV recognizes the carcinogenic potential of PPAH collectively].

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/284 = 246$ ug/m^3
Water, Health: $15 \times 2.46 \times 10^2 = 3.70 \times 10^3$ ug/ℓ
Land, Health: $0.2 \times 3.70 \times 10^3 = 740$ ug/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 284) = 0.59$ ug/m^3
$EPC_{WC} = 15 \times 0.59 = 8.85$ ug/ℓ
$EPC_{LC} = 0.2 \times 8.85 = 1.77$ ug/g

MULTIMEDIA ENVIRONMENTAL GOALS

X
23B220
DIBENZ(a,j)ACRIDINE

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			2.5E2		0.59		4×10^{-5}†
Water, μg/l (ppm Wt)			3.7E3		8.85		
Land, μg/g (ppm Wt)			7.4E2		1.77		

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)					0.59
Water, μg/l (ppm Wt)					8.85
Land, μg/g (ppm Wt)					1.77

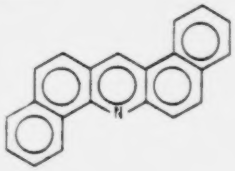
† Reported for urban atmosphere. No rural concentration is reported.

CATEGORY: 23B

WLN: T G6 D6 B666 CNJ

DIBENZ(a,h)ACRIDINE: $C_{21}H_{13}N$. (1,2:5,6-Dibenzacridine). 23B240

STRUCTURE:



Dibehz(a,h)acridine is obtained as yellow crystals from ethanol; solutions of the compound exhibit fluorescence.

PROPERTIES:

Molecular wt: 279.34; mp: 228; solubility in water may be enhanced by the presence of acids as impurities in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Acridines may be found in coal tar and pitch. They are associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 8). The average atmospheric urban concentration of dibenz(a,h)acridine in the United States is reported as 0.08 μg/1,000 m^3 air (ref. 14).

The acridines are classified as weak bases.

TOXIC PROPERTIES, HEALTH EFFECTS:

Dibenz(a,h)acridine may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man (refs. 7, 10). Dibenz(a,h)acridine is reported to cause tumors in mice. The EPA/NIOSH ordering number is 3124. The lowest toxic dose to induce a carcinogenic response is 10 mg.kg (ref. 13). The adjusted ordering number is 312.4

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 [for particulate polycyclic aromatic hydrocarbons (PPAH). This TLV recognizes the carcinogenic potential of PPAH collectively].

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/312.4 = 224$ $\mu g/m^3$

Water, Health: $15 \times 224 = 3.36 \times 10^3$ $\mu g/\ell$

Land, Health: $0.2 \times 3.36 \times 10^3 = 672$ $\mu g/g$

Air, Ecology:

Water, Ecology:

Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 312.4) = 0.53$ $\mu g/m^3$

$EPC_{WC} = 15 \times 0.53 = 8.0$ $\mu g/\ell$

$EPC_{LC} = 0.2 \times 8.0 = 1.6$ $\mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

X
23B240
DIBENZ(a,h)ACRIDINE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.2E2		0.53		8×10^{-5}†
Water, $\mu g/l$ (ppm Wt)			3.4E3		8.0		
Land, $\mu g/g$ (ppm Wt)			6.7E2		1.6		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					0.5
Water, $\mu g/l$ (ppm Wt)					8.0
Land, $\mu g/g$ (ppm Wt)					1.6

†Reported for urban atmosphere. No rural concentration is reported.

CATEGORY: 23B

DIBENZ(c,h)ACRIDINE: $C_{21}H_{13}N$ (3,4:5,6-dibenzacridine). 23B260
Dibenz(c,h)acridine is obtained as yellow crystals from ethanol. Solutions of the compound exhibit fluorescence.

PROPERTIES:

Molecular wt.: 279.35; mp: 189; sublimes; solubility in water may be enhanced by the presence of acids as impurities in water.

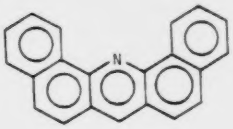
NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Acridines may be found in coal tar and pitch. They are associated with particulate polycyclic aromatic hydrocarbons, PPAH (ref. 8).

The acridines are classified as weak bases.

WLN: T E6 D6 B666 CNJ

STRUCTURE:



TOXIC PROPERTIES, HEALTH EFFECTS:

Dibenz(c,h)acridine may be present in soot, coal tar, and pitch, which are known to be carcinogenic to man (refs. 7, 10). Although not considered to be a highly active carcinogen alone, dibenz(c,h) acridine is reported to cause tumors in mice. The EPA/NIOSH ordering number is 3122. The lowest dose to induce an oncogenic response is reported as 1,020 mg/kg (ref. 13). The adjusted ordering number is 3.06.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 [for particulate polycyclic aromatic hydrocarbons (PPAH). This TLV recognizes the carcinogenic potential of PPAH collectively].

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/3.06 = 2.3 \times 10^4$ μg/m^3
Water, Health: $15 \times 2.3 \times 10^4 = 3.45 \times 10^5$ μg/ℓ
Land, Health: $0.2 \times 3.45 \times 10^5 = 6.9 \times 10^4$ μg/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 3.06) = 54.5$ μg/m^3
$EPC_{WC} = 15 \times 54.5 = 817.5$ μg/ℓ
$EPC_{LC} = 0.2 \times 817.5 = 163.5$ μg/g

339<

MULTIMEDIA ENVIRONMENTAL GOALS

23B260
DIBENZ(c,h)ACRIDINE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.3E4		54.5		
Water, $\mu g/l$ (ppm Wt)			3.5E5		817		
Land, $\mu g/g$ (ppm Wt)			6.9E4		163		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					54.5
Water, $\mu g/l$ (ppm Wt)					817
Land, $\mu g/g$ (ppm Wt)					163

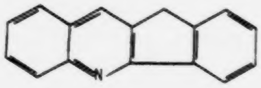
400<

CATEGORY: 23B

2,3-BENZ-4-AZAFLUORENE: $C_{16}H_{11}N$ (11-Indeno(1,2-b) quinoline). 23B280
Colorless needles from benzene.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 217.28; mp: 169-70; bp: 412.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

2,3-Benz-4-azafluorene is a constituent of anthracite pitch. It is associated with particulate polycyclic organic matter (ref. 8).

TOXIC PROPERTIES, HEALTH EFFECTS:

No information is available regarding toxic effects or carcinogenic potential for this compound alone.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	Air, Ecology:
Water, Health:	Water, Ecology:
Land, Health:	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

23B280
2,3-BENZ-4-AZAFLUORENE

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

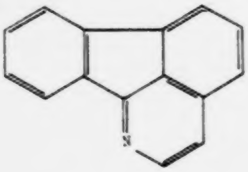
	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

CATEGORY: 23B

INDENO(1,2,3-ij)ISOQUINOLINE: $C_{15}H_9N$ 23B300
(2-azafluoranthene).
Pale yellow crystals.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 203.25 mp: 91-92.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Indeno(1,2,3-ij)isoquinoline has been reported in airborne particulates and gasoline exhaust (ref. 8). Acidic solvents are used to extract the compound from the particulate matter for qualitative and quantitative identification (ref. 8).

Indeno(1,2,3-ij)isoquinoline is likely to be associated with particulate polycyclic aromatic hydrocarbons. The compound has been isolated from coal tar (ref. 18).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological properties for indeno(1,2,3-ij)isoquinoline are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m³ (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA
ENVIRONMENTAL
GOALS

23B300

INDENO(1,2,3-ij)ISOQUINOLINE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
Category	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

REFERENCES: CATEGORY 23B

Heterocyclic Nitrogen Compounds - Fused Six-Membered Ring Heterocycles

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465<

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CATEGORY 23

HETEROCYCLIC NITROGEN COMPOUNDS

SUBCATEGORY: 23C - Pyrrole and Fused Ring Derivatives of Pyrrole

Summary of Subcategory

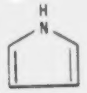
Total number of compounds in subcategory	11
number of parent compounds with subspecies	2
number of subspecies	4
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	5

Consent Decree compounds included in subcategory: 0

CATEGORY: 23C

WLN: TSMJ

STRUCTURE:



PYRROLE: C_4H_5N (1-aza-2,4-cyclopentadiene, azole, divinyleneimine). 23C020
Colorless liquid when freshly distilled, darkens on exposure to air, odor similar to that of chloroform.

PROPERTIES:

Molecular wt: 67.09; bp: 130; d: 0.9691^{20}_{4}; vap. d.: 2.31; pK_b: 13.6 (ref. 1); sparingly soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Pyrrole occurs in coal tar and bone oil. It is produced in coal carbonization (ref. 4). The pyrrole ring is part of important, naturally occurring compounds, including haemin, chlorophyll, bile pigments, and many alkaloids (refs. 2,3).

TOXIC PROPERTIES, HEALTH EFFECTS:

Pyrrole is generally regarded as having a low degree of toxicity (ref. 1).
LD_{50} (subcutaneous, mouse): 61 mg/kg.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 61 = 2.7 \times 10^3$ μg/m^3
Water, Health: $15 \times 2.7 \times 10^3 = 4.05 \times 10^4$ μg/ℓ
Land, Health: $0.2 \times 4.05 \times 10^4 = 8,100$ μg/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 61 = 6.5$ μg/m^3
$EPC_{AH3} = 0.081 \times 61 = 5$ μg/m^3
$EPC_{WH1} = 15 \times 5 = 75$ μg/ℓ
$EPC_{WH2} = 0.4 \times 61 = 24$ μg/ℓ
$EPC_{LH} = 0.2 \times 24 = 4.8$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

23C020
PYRROLE

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.7E3		5		
Water, $\mu g/l$ (ppm Wt)			4.1E4		24		
Land, $\mu g/g$ (ppm Wt)			8.1E3		4.8		

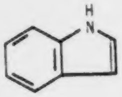
*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			5		
Water, $\mu g/l$ (ppm Wt)			24		
Land, $\mu g/g$ (ppm Wt)			4.8		

CATEGORY: 23C **WLN:** T56 BMJ

INDOLE: C_8H_7N (2,3-benzopyrrole, 1-azaindene, 1-benzazole). 23C040 **STRUCTURE:**
Colorless leaflets from water. Pleasant odor when pure.



PROPERTIES:

Molecular wt: 117.15; mp: 52; bp: 253-4;
soluble in hot water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Indole occurs in coal tar, in jasmine, orange blossom, and other flower oils, and with skatole in feces (ref. 2). Indole-3-acetic acid is an important plant growth hormone (ref. 5).

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{50} (oral, rat): 1,000 mg/kg.

Indole is reported to cause tumors in mice. The EPA/NIOSH ordering number is 3121. The lowest dose to induce an oncogenic response is reported as 480 mg/kg. The adjusted ordering number is 6.5.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/6.5 = 1.1 \times 10^4\ \mu g/m^3$	Air, Ecology:
Water, Health: $15 \times 1.1 \times 10^4 = 1.65 \times 10^5\ \mu g/\ell$	Water, Ecology:
Land, Health: $0.2 \times 1.65 \times 10^5 = 3.3 \times 10^4\ \mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 1,000 = 107\ \mu g/m^3$
$EPC_{AH3} = 0.081 \times 1,000 = 81\ \mu g/m^3$
$EPC_{WH1} = 15 \times 31 = 1,200\ \mu g/\ell$
$EPC_{WH2} = 0.4 \times 1,000 = 400\ \mu g/\ell$
$EPC_{LH} = 0.2 \times 400 = 80\ \mu g/g$
$EPC_{AC2} = 10^3/(6 \times 6.5) = 26\ \mu g/m^3$
$EPC_{WC} = 15 \times 26 = 390\ \mu g/\ell$
$EPC_{LC} = 0.2 \times 390 = 78\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

23C040 INDOLE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.1E4		26		
Water, $\mu g/l$ (ppm Wt)			1.7E5		390		
Land, $\mu g/g$ (ppm Wt)			3.3E4		78		

*To be multiplied by dilution factor

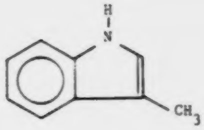
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			81		26
Water, $\mu g/l$ (ppm Wt)			400		390
Land, $\mu g/g$ (ppm Wt)			80		78

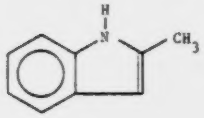
CATEGORY: 23C

METHYLINDOLES: C_9H_9N 23C060
2-METHYLINDOLE: A solid. 23C061
3-METHYLINDOLE: (skatole). White to brownish scales with fecal odor. 23C062

WLN:

STRUCTURE:





PROPERTIES:

	mol.wt.	mp.	bp.	d.	solubility in water
2-methylindole	131.18	61	272	1.07_4^{20}	soluble when hot
3-methylindole	131.18	97-8	$265\text{-}6^{755}$		soluble

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

3-Methylindole is a natural constituent of feces, beet root, nectandra wood, and coal tar (ref. 6).

Methylindole is likely to be associated with particulate polycyclic aromatic hydrocarbons and has been identified in the ambient air of Rome, Italy at a concentration of 2 ng/m^3 (ref. 7).

Threshold odor concentration for 3-methylindole is reported as 0.0004 μg/m^3 (ref. 8).

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{Lo} (subcutaneous, frog): 1,000 mg/kg for 3-methylindole (ref. 9).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 1{,}000 = 4.5 \times 10^4$ μg/m^3

Water, Health: $15 \times 4.5 \times 10^4 = 6.75 \times 10^5$ μg/l

Land, Health: $0.2 \times 6.75 \times 10^5 = 1.35 \times 10^5$ μg/g

Air, Ecology:

Water, Ecology:

Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 1{,}000 = 107$ μg/m^3

$EPC_{AH3} = 0.081 \times 1{,}000 = 81$ μg/m^3

$EPC_{WH1} = 15 \times 81 = 1{,}215$ μg/l

$EPC_{WH2} = 0.4 \times 1{,}000 = 400$ μg/l

$EPC_{LH} = 0.2 \times 400 = 80$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

23C060
METHYLINDOLES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			4.5E4		81		
Water, $\mu g/l$ (ppm Wt)			6.8E5		400		
Land, $\mu g/g$ (ppm Wt)			1.4E5		80		

*To be multiplied by dilution factor

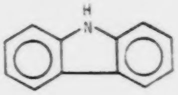
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			81		
Water, $\mu g/l$ (ppm Wt)			400		
Land, $\mu g/g$ (ppm Wt)			80		

CATEGORY: 23C

WLN: T B656 HMJ

CARBAZOLE: $C_{12}H_9N$ (9-azafluorene, dibenzo(b,d)pyrrole, diphenyleneimine). 23C080
Colorless, slightly fluorescent plates.

STRUCTURE:



PROPERTIES:

Molecular wt: 167.20; mp: 245; bp: 355; d: 1.10_4^{18}; vap. press: 400 mm at 323°; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Carbazole occurs in anthracene oil of coal tar. Simple substituted carbazoles have been isolated from plants (ref. 5). It is a weaker base than diphenylamine (ref. 2).

Carbazole is associated with particulate polycyclic organic matter (ref. 10) and has been identified in the ambient air of Rome, Italy, in concentrations up to 1.1 ng/m^3.

TOXIC PROPERTIES, HEALTH EFFECTS:

Carbazole is a known allergen (ref. 11).

LD_{Lo} (oral, rat): 500 mg/kg.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 500 = 2.25 \times 10^4$ μg/m^3
Water, Health: $15 \times 2.25 \times 10^4 = 3.4 \times 10^5$ μg/ℓ
Land, Health: $0.2 \times 3.4 \times 10^5 = 6.8 \times 10^4$ μg/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 500 = 54$ μg/m^3
$EPC_{AH3} = 0.081 \times 500 = 41$ μg/m^3
$EPC_{WH1} = 15 \times 41 = 615$ μg/ℓ
$EPC_{WH2} = 0.4 \times 500 = 200$ μg/ℓ
$EPC_{LH} = 0.2 \times 200 = 40$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

23C080 CARBAZOLE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			2.3E4		41		
Water, μg/l (ppm Wt)			3.5E5		200		
Land, μg/g (ppm Wt)			6.8E4		40		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			41		
Water, μg/l (ppm Wt)			200		
Land, μg/g (ppm Wt)			40		

CATEGORY: 23C

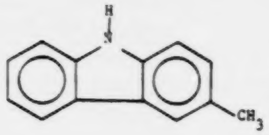
WLN:

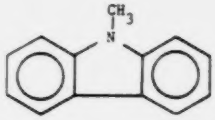
METHYLCARBAZOLES: $C_{13}H_{11}N$(methyldibenzopyrrole, methyldiphenylenimine). 23C100

3-METHYLCARBAZOLE: (3-methyldibenzopyrrole, 3-methyldiphenylenimine). A solid. 23C101

9-METHYLCARBAZOLE: (9-methyldibenzopyrrole, 9-methyldiphenylenimine). A solid. 23C102

STRUCTURE:





PROPERTIES:

	mol.wt	mp.	bp.	solubility in water
9-methylcarbazole	181.24	88	195^{12}	insoluble
3-methylcarbazole	181.24			

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Substituted carbazoles occur naturally in the Rutaceae family, and the majority of compounds have been isolated from a single plant species (ref. 5).

Carbazole and its methyl derivatives have been reported to be present in urban atmosphere. Possible sources are fumes of coal-tar pitch (ref. 10). Methylcarbazoles are likely to be associated with particulate polycyclic aromatic hydrocarbons.

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for methylcarbazoles are not available at this time. However, toxicological characteristics of methylcarbazoles are likely to be similar to those of carbazole because of the chemical structure similarity.

Substance	LD_{50}(oral,rat) (mg/kg)	Methylated Substance	LD_{50}(oral,rat) (mg/kg)	LD_{Lo} (subcutaneous, frog) (mg/kg)
Pyridine	891	methylpyridine	800	
Quinoline	460	methylquinoline	1,230	
Indole	1,000	methylindole		1,000
Carbazole	500			

The available data indicate that methylation of these similar compounds does not increase the toxicity of the compound.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m³ (for particulate polycyclic aromatic hydrocarbons (PPAH). This TLV recognizes the carcinogenic potential of PPAH collectively.)

***MINIMUM ACUTE TOXICITY CONCENTRATIONS**:

Air, Health: $45 \times 500 = 2.25 \times 10^4\ \mu g/m^3$ Air, Ecology:

Water, Health: $15 \times 2.25 \times 10^4 = 3.4 \times 10^5\ \mu g/l$ Water, Ecology:

Land, Health: $0.2 \times 3.4 \times 10^5 = 6.8 \times 10^4\ \mu g/g$ Land, Ecology:

***ESTIMATED PERMISSIBLE CONCENTRATIONS**:

$EPC_{AH1} = 0.107 \times 500 = 54\ \mu g/m^3$

$EPC_{AH2} = 0.081 \times 500 = 41\ \mu g/m^3$

$EPC_{WH1} = 15 \times 41 = 615\ \mu g/l$

$EPC_{WH2} = 0.4 \times 500 = 200\ \mu g/l$

$EPC_{LH} = 0.2 \times 200 = 40\ \mu g/g$

*Based on LD_{50} (oral, rat): 500 mg/kg for carbazole.

MULTIMEDIA ENVIRONMENTAL GOALS

23C100
METHYLCARBAZOLES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent †		B. Ambient Level Goal* †		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.3E4		41		
Water, $\mu g/l$ (ppm Wt)			3.4E5		200		
Land, $\mu g/g$ (ppm Wt)			6.8E4		40		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration †		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			41		
Water, $\mu g/l$ (ppm Wt)			200		
Land, $\mu g/g$ (ppm Wt)			40		

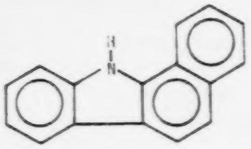
† Based on data for carbazole.

CATEGORY: 23C

BENZO(a)CARBAZOLE: $C_{16}H_{11}N$ (1,2-benzcarbazole, 11 H-benzo(a)carbazole). 23C120
A solid.

WLN: T D6 B566 CMJ

STRUCTURE:



PROPERTIES:

Molecular wt: 217.28; mp:228; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Carbazoles are generally weak bases (ref. 2). Simple substituted carbazoles have been isolated from plants (ref. 5).

Benzo(a)carbazole may be associated with particulate polycyclic organic matter. Benzocarbazoles are reported to occur in air containing fumes of coal-tar pitch (ref. 10).

TOXIC PROPERTIES, HEALTH EFFECTS:

Benzo(a)carbazole is a carcinogen in the mouse (ref. 9). The EPA/NIOSH ordering number is 3,121. The lowest dose to induce a carcinogenic response is 840 mg/kg. The adjusted ordering number is 3.7.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m³ (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively.)

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$7 \times 10^4/3.7 = 1.89 \times 10^4\ \mu g/m^3$	Air, Ecology:
Water, Health:	$15 \times 1.89 \times 10^4 = 2.84 \times 10^5\ \mu g/l$	Water, Ecology:
Land, Health:	$0.2 \times 2.84 \times 10^5 = 5.68 \times 10^4\ \mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 3.7) = 45.0\ \mu g/m^3$

$EPC_{WC} = 15 \times 45.0 = 675\ \mu g/l$

$EPC_{LC} = 0.2 \times 675 = 135\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

23C120

BENZO(a)CARBAZOLE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.9E4		45		
Water, $\mu g/l$ (ppm Wt)			2.8E5		675		
Land, $\mu g/g$ (ppm Wt)			5.7E4		135		

*To be multiplied by dilution factor

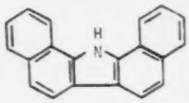
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					45
Water, $\mu g/l$ (ppm Wt)					675
Land, $\mu g/g$ (ppm Wt)					135

CATEGORY: 23C

WLN: T E6 D6 B566 CMJ

DIBENZO(a,i)CARBAZOLE: $C_{20}H_{13}N$ (7H-dibenzo(a,i)carbazole, 1,2:7,8-dibenzocarbazole). 23C140
Colorless leaflets from acetic acid.

STRUCTURE:



PROPERTIES:

Molecular wt: 267.34; mp: 221; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Carbazoles are in general weak bases (ref. 2). Simple substituted carbazoles have been isolated from plants (ref. 5).

The compound may be associated with particulate polycyclic organic matter.

TOXIC PROPERTIES, HEALTH EFFECTS:

Dibenzo(a,i)carbazole is reported to cause tumors in mice. The EPA/NIOSH ordering number is 3121. The lowest toxic dose to induce an oncogenic response is reported as 510 mg/kg. The adjusted ordering number is 6.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/6 = 1.2 \times 10^4$ $\mu g/m^3$	Air, Ecology:
Water, Health: $15 \times 1.2 \times 10^4 = 1.8 \times 10^5$ $\mu g/\ell$	Water, Ecology:
Land, Health: $0.2 \times 1.8 \times 10^5 = 3.6 \times 10^4$ $\mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 6) = 28$ $\mu g/m^3$
$EPC_{WC} = 15 \times 28 = 420$ $\mu g/\ell$
$EPC_{LC} = 0.2 \times 420 = 84$ $\mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

23C140
DIBENZO(a,i)CARBAZOLE

EMISSION [illegible]EL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.2E4		28		
Water, $\mu g/l$ (ppm Wt)			1.8E5		420		
Land, $\mu g/g$ (ppm Wt)			3.6E4		84.0		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					28
Water, $\mu g/l$ (ppm Wt)					420
Land, $\mu g/g$ (ppm Wt)					84.0

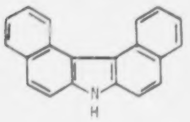
CATEGORY: 23C

DIBENZO(c,g)CARBAZOLE: $C_{20}H_{13}N$ (7H-Dibenzo(c,g)carbazole, 3,4:5,6-dibenzocarbazole). 23C160

Colorless needles from ethanol.

WLN: T D6 C6 B566 MMJ

STRUCTURE:



PROPERTIES:

Molecular wt: 267.34; mp: 158; insoluble in water; lipid solubility: 0.3 mg/0.25 ml tricaprylin (ref. 12).

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Carbazoles are, in general, weak bases (ref. 2). Simple substituted carbazoles have been isolated from plants (ref. 5).

Dibenzo(c,g)carbazole is associated with particulate polycyclic organic matter (ref. 10).

TOXIC PROPERTIES, HEALTH EFFECTS:

Dibenzo(c,g)carbazole is a carcinogen in the mouse, rat, hamster, and possibly in the dog (ref. 12). The EPA/NIOSH ordering number is 5429. The lowest dose to induce a carcinogenic response is reported as 8 mg/kg. The adjusted ordering number is 679.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/679 = 103\ \mu g/m^3$
Water, Health: $15 \times 103 = 1.5 \times 10^3\ \mu g/\ell$
Land, Health: $0.2 \times 1.5 \times 10^3 = 300\ \mu g/g$

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 679) = 0.24\ \mu g/m^3$
$EPC_{WC} = 15 \times 0.24 = 3.6\ \mu g/\ell$
$EPC_{LC} = 0.2 \times 3.5 = 0.72\ \mu g/g$

MULTIMEDIA ENVIRONMENTAL GOALS

X
23C160
DIBENZO(c,g)CARBAZOLE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			1.0E2		0.2		
Water, $\mu g/l$ (ppm Wt)			1.5E3		3.6		
Land, $\mu g/g$ (ppm Wt)			3.0E2		0.7		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					0.2
Water, $\mu g/l$ (ppm Wt)					3.6
Land, $\mu g/g$ (ppm Wt)					0.7

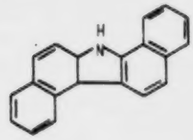
423<

CATEGORY: 23C

WLN: T F6 C6 B566 MMJ

DIBENZO(a,g)CARBAZOLE: $C_{20}H_{13}N$ (7H-dibenzo(a,g)-carbazole, 1,2:5,6-dibenzocarbazole). 23C180
Colorless needles from acetone.

STRUCTURE:



PROPERTIES:

Molecular wt: 267.34; mp: 231; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Carbazoles are in general weak bases (ref. 2). Simple substituted carbazoles have been isolated from plants (ref. 5). The compound may be associated with particulate polycyclic organic matter.

TOXIC PROPERTIES, HEALTH EFFECTS:

Dibenzo(a,g)carbazole is reported to cause tumors in mice. The EPA/NIOSH ordering number is 3121. The lowest dose to induce a carcinogenic response is 270 mg/kg. The adjusted ordering number is 11.6.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV = 0.2 mg/m^3 (for particulate polycyclic aromatic hydrocarbons [PPAH]. This TLV recognizes the carcinogenic potential of PPAH collectively).

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $7 \times 10^4/11.6 = 6 \times 10^3$ µg/m^3	Air, Ecology:
Water, Health: $15 \times 6 \times 10^3 = 9 \times 10^4$ µg/ℓ	Water, Ecology:
Land, Health: $0.2 \times 9 \times 10^4 = 1.8 \times 10^4$ µg/g	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AC2} = 10^3/(6 \times 11.6) = 14$ µg/m^3
$EPC_{WC} = 15 \times 14 = 210$ µg/ℓ
$EPC_{LC} = 0.2 \times 210 = 42$ µg/g

MULTIMEDIA ENVIRONMENTAL GOALS

23C180
DIBENZO(a,g)CARBAZOLE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			6.0E3		14		
Water, $\mu g/l$ (ppm Wt)			9.0E4		210		
Land, $\mu g/g$ (ppm Wt)			1.8E4		42		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					14
Water, $\mu g/l$ (ppm Wt)					210
Land, $\mu g/g$ (ppm Wt)					42

REFERENCES: CATEGORY 23C

Heterocyclic Nitrogen Compounds - Pyrrole and Fused Ring Derivatives of Pyrrole

1. Sutton, W. L. Heterocyclic and Miscellaneous Nitrogen Compounds. Industrial Hygiene and Toxicology, Second Revised Edition, Vol. 2, F. A. Patty, Ed., Interscience Publishers, New York, NY (1963).

2. Livingstone, R. Compounds Containing a Five-Membered Ring with One Hetero Atom from Group V: Nitrogen--Fused-Ring Compounds. Rodd's Chemistry of Carbon Compounds, Second Edition, Vol. 4, Part A, S. Coffey, Ed., Elsevier Scientific Publishing Company, Amsterdam (1973).

3. Smith, K. M. The Pyrrole Pigments. Rodd's Chemistry of Carbon Compounds, Second Edition, Vol. 4, Part B: Heterocyclic Compounds, S. Coffey, Ed., Elsevier Scientific Publishing Company, Amsterdam (1973).

4. Braunstein, H. M., E. D. Copenhauer, and H. A. Pfuderer (Eds.). Environmental, Health, and Control Aspects of Coal Conversion: An Information Overview. Oak Ridge National Laboratory, Oak Ridge TN 37830. Prepared for the Energy Research and Development Administration, April 1977.

5. Stapleford, K. S. J. The Indole Alkaloids. Rodd's Chemistry of Carbon Compounds, Second Edition, Vol. 4, Part B, S. Coffey, Ed., Elsevier Scientific Publishing Company, Amsterdam (1973).

6. Windholz, M., Ed. The Merck Index: An Encyclopedia of Chemicals and Drugs, Ninth Edition. Merck & Co., Inc., Rahway, NJ (1976).

7. Kingsbury, G. L., R. C. Sims, and J. B. White. Source and Ambient Concentration Data for Polycyclic Organic Matter. Vol. I-III. Draft of Report Prepared by Research Triangle Institute, under Contract No. 68-02-2612 for U.S. Environmental Protection Agency. Available from J. O. Milliken, Project Officer, IERL-EPA, Research Triangle Park, N.C. (1978).

8. Verschueren, K. Handbook of Environmental Data on Organic Chemicals. Van Nostrand Rheinhold Company, NY (1977).

9. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

10. U.S. Environmental Protection Agency, Office of Research and Development. Scientific and Technical Assessment Report on Particulate Polycyclic Organic Matter (PPOM). Star Series. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC EPA-600/6-74-001 (1975).

REFERENCES: CATEGORY 23C (Continued)

11. Sax, N. I., Ed. Dangerous Properties of Industrial Materials, Fourth Edition. Van Nostrand Reinhold Co., New York, NY (1975).

12. International Agency for Research on Cancer. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Man, Vol. 3, Lyon, France. A World Health Organization Publication (WHO), Geneva (1973).

CATEGORY 23

HETEROCYCLIC NITROGEN COMPOUNDS

SUBCATEGORY: 23D - Nitrogen Heterocycles Containing Additional Hetero Atoms

Summary of Subcategory

Total number of compounds in subcategory	2
number of parent compounds with subspecies	0
number of subspecies	0
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

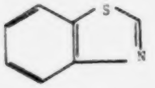
Consent Decree compounds included in subcategory: 0

CATEGORY: 23D

BENZOTHIAZOLE: C_7H_5NS (benzosulfonazole).
A liquid with the odor of quinoline. 23D020

WLN: T56 BN DSJ

STRUCTURE:



PROPERTIES:

Molecular wt: 135.19; mp:2; bp:231^{760}; d:1.2460_4^{20};
slightly soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzothiazole can be formed from the reaction between N,N-dimethylaniline and sulfur (ref. 1).

Benzothiazole has been reported in samples taken from finished drinking water (ref. 2) and in urban air (ref. 3).

Benzothiazole is used in the manufacture of photographic dyes and rubber chemicals (ref. 4).

TOXIC PROPERTIES, HEALTH EFFECTS:

LD_{50} (intravenous,mouse): 95 mg/kg (ref. 5).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$45 \times 95 = 4{,}275$ µg/m^3	Air, Ecology:
Water, Health:	$15 \times 4{,}275 = 6.41 \times 10^4$ µg/l	Water, Ecology:
Land, Health:	$0.2 \times 6.41 \times 10^4 = 1.28 \times 10^4$ µg/g	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 95 = 10.2$ µg/m^3

$EPC_{AH3} = 0.081 \times 95 = 7.70$ µg/m^3

$EPC_{WH1} = 15 \times 7.70 = 115.5$ µg/l

$EPC_{WH2} = 0.4 \times 95 = 38$ µg/l

$EPC_{LH} = 0.2 \times 38 = 7.6$ µg/g

MULTIMEDIA ENVIRONMENTAL GOALS

23D020
BENZOTHIAZOLE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			4.3E3		7.7		
Water, $\mu g/l$ (ppm Wt)			6.4E4		38		
Land, $\mu g/g$ (ppm Wt)			1.3E4		7.6		

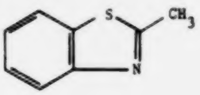
*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			7.7		
Water, $\mu g/l$ (ppm Wt)			38		
Land, $\mu g/g$ (ppm Wt)			7.6		

CATEGORY: 23D
2-METHYL BENZOTHIAZOLE: C_8H_7NS 23D040
A colorless liquid with an odor similar to pyridine.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 149.22; mp: 14; bp: 240; d: $1.1763_4^{19.4}$; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

2-Methyl benzothiazole has been reported in samples taken from finished drinking water (ref. 2).

2-Methyl benzothiazole is used in the syntheses of dyes, and in the syntheses of dye bases for use as pH indicators (ref. 6).

The compound has been reported to be microbiologically synthesized by cultures of cordyceps militaris (ref. 7).

The 2,6-diamino analogue of 2-methyl benzothiazole is almost as effective as the antibiotic streptomycin in guinea pigs (ref. 8).

TOXIC PROPERTIES, HEALTH EFFECTS:

2-Methyl benzothiazole has been tested for bacteriostatic effects against tubercle bacilli in vivo and in guinea pigs, and has demonstrated weak activity (ref. 5).

LD_{50} (intravenous, mouse): 105 mg/kg

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$45 \times 105 = 4{,}725\ \mu g/m^3$	Air, Ecology:
Water, Health:	$15 \times 4{,}725 = 7.09 \times 10^4\ \mu g/l$	Water, Ecology:
Land, Health:	$0.2 \times 7.09 \times 10^4 = 1.42 \times 10^4\ \mu g/g$	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 105 = 11.24\ \mu g/m^3$

$EPC_{AH3} = 0.081 \times 105 = 8.51\ \mu g/m^3$

$EPC_{WH1} = 15 \times 8.51 = 127.7\ \mu g/l$

$EPC_{WH2} = 0.4 \times 105 = 42\ \mu g/l$

$EPC_{LH} = 0.2 \times 42 = 8.4\ \mu g/g$

23D040
2-METHYL BENZOTHIAZOLE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			4.7E3		8.5		
Water, $\mu g/l$ (ppm Wt)			7.1E4		42		
Land, $\mu g/g$ (ppm Wt)			1.4E4		8		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			8.5		
Water, $\mu g/l$ (ppm Wt)			42		
Land, $\mu g/g$ (ppm Wt)			8		

REFERENCES: CATEGORY 23D

Heterocyclic Nitrogen Compounds - Nitrogen Heterocycles Containing Additional Hetero Atoms

1. Windholz, M., Ed. The Merck Index: An Encyclopedia of Chemicals and Drugs, Ninth Edition. Merck & Co., Inc., Rahway, NJ (1976).

2. Shackelford, W. M., and L. H. Keith. Frequency of Organic Compounds Identified in Water. EPA Publication No. 600/4-76-062, December 1976.

3. Kingsbury, G. L., R. C. Sims, and J. B. White. Source and Ambient Concentration Data for Polycyclic Organic Matter. Vol. I-III. Draft of Report Prepared by Research Triangle Institute, under Contract No. 68-02-2612 for U.S. Environmental Protection Agency. Available from J. O. Milliken, Project Officer, IERL-EPA, Research Triangle Park, N.C. (1978).

4. Verschueren, K. Handbook of Environmental Data on Organic Chemicals. Van Nostrand Rheinhold Company, NY (1977).

5. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

6. Rodd, E. H. Chemistry of Carbon Compounds, Vol. IV, Part B, Elsevier Scientific Publishing Company, Inc., New York, NY (1965).

7. Mutschler, E. Archives Pharmacology 300: 695 (1967).

8. Freedlanker, B. Proceedings of the Society of Experimental Biology 66: 3625 (1947).

CATEGORY 24

HETEROCYCLIC OXYGEN COMPOUNDS

SUBCATEGORY: 24A - One- and Two-Ring Heterocyclic Oxygen Compounds

Summary of Subcategory

Total number of compounds in subcategory	6
number of parent compounds with subspecies	1
number of subspecies	4
Number of parent compounds with no MEG values	2
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

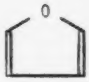
Consent Decree compounds included in subcategory: 0

CATEGORY: 24A

WLN:

FURAN: C_4H_4O (furfurane, oxole, tetrole, divinylene oxide).
A colorless liquid. 24A020

STRUCTURE:



PROPERTIES:

Molecular wt: 68.08; mp: -85.65; bp: 31.36^{760}; d: 0.9514^{20}_{4}; vap.d: 2.35; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Furan occurs in oils obtained by the distillation of resin containing pine wood. It can be formed by decarboxylation of 2-furancarboxylic acid (ref. 1).

Unstabilized, furan may form unstable peroxides on exposure to air. Contact with acids may initiate a violent exothermic reaction (ref. 2).

Furan is a heterocycle that is considered an aromatic compound on the basis of its properties. The structural formula does not adequately represent the structure of the compound.

TOXIC PROPERTIES, HEALTH EFFECTS:

Furan has narcotic and analgesic properties. It is highly toxic if inhaled and is absorbed through the skin. Symptoms include convulsions followed by paralysis of the respiratory center and asphyxia (ref. 3).

LC_{Lo} (inhalation, rat): 84,500 mg/m^3 for 8-48 hours, continuous (ref. 4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	84,500 x 100 = 8.45×10^6 μg/m^3	Air, Ecology:
Water, Health:	15 x 8.45×10^6 = 1.26×10^8 μg/ℓ	Water, Ecology:
Land, Health:	0.2 x 1.26×10^8 = 2.54×10^7 μg/g	Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

435<

MULTIMEDIA ENVIRONMENTAL GOALS

24A020 FURAN

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			8.5E6				
Water, $\mu g/l$ (ppm Wt)			1.3E8				
Land, $\mu g/g$ (ppm Wt)			2.5E7				

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

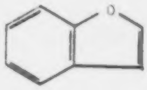
CATEGORY: 24A

BENZOFURAN: C_8H_6O (coumarone, cumarone) 24A040

An oily liquid with an aromatic odor.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 118.14; mp:<-18; bp:174^{760}; d:1.0913^{23}; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzofuran is a constituent of coal tar; it has been isolated from coal tar oils (ref. 1).

Benzofuran used in the manufacturing of coumarone-indene resins is derived from the crude heavy solvent naphtha fraction of coal tar light oil, which is obtained as a byproduct in the coking of bituminous coal (ref. 1).

Benzofuran has been reported in gasoline exhaust at concentrations from <0.1 ppm to 2.8 ppm (ref. 4).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for benzofuran are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

24A040
BENZOFURAN

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSFS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

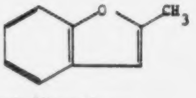
*To be multiplied by dilution factor

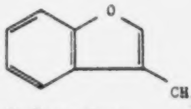
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

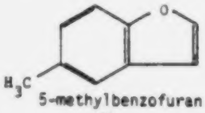
CATEGORY: 24A
METHYLBENZOFURANS: C_9H_8O 24A060
2-METHYLBENZOFURAN: A liquid. 24A061
3-METHYLBENZOFURAN: A liquid. 24A062
5-METHYLBENZOFURAN: A liquid. 24A063
7-METHYLBENZOFURAN: A liquid. 24A064

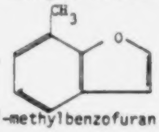
WLN:

STRUCTURE:


2-methylbenzofuran


3-methylbenzofuran


5-methylbenzofuran


7-methylbenzofuran

PROPERTIES:

	mol. wt.	bp.	d.	solubility in water
2-methylbenzofuran:	132.17	$197.3-.8^{760}$	1.0540^{20}_{4}	insoluble
3-methylbenzofuran:	132.17	$196-7^{742}$	1.0540^{23}_{4}	insoluble
5-methylbenzofuran:	132.17	197-9	1.0603^{19}	insoluble
7-methylbenzofuran:	132.17	190-1	1.0490^{19}	insoluble

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

It is likely that methylbenzofurans are associated with particulate polycyclic aromatic hydrocarbons (ref. 6).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for methylbenzofurans are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

24A060
METHYLBENZOFURANS

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
Category	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

REFERENCES: CATEGORY 24A

Heterocyclic Oxygen Compounds - One- and Two-Ring Heterocyclic Oxygen Compounds

1. Windholz, M., Ed. The Merck Index: An Encyclopedia of Chemicals and Drugs, Ninth Edition. Merck & Co., Inc., Rahway, NJ (1976).

2. Sax, N. I., Ed. Dangerous Properties of Industrial Materials, Fourth Edition. Van Nostrand Reinhold Co., New York, NY (1975).

3. Browning, Ethel. Toxicity and Metabolism of Industrial Solvents. Elsevier Publishing Company, London, 1965.

4. Spector, W. S. (Ed.). Handbook of Toxicology, Volume I, W. B. Saunders Company, Philadelphia and London. Prepared under the direction of the Committee on the Handbook of Biological Data, Division of Biology and Agriculture, the National Academy of Sciences, and the National Research Council. 1956-1959.

5. Verschueren, K. Handbook of Environmental Data on Organic Chemicals. Van Nostrand Reinhold Company, NY (1977).

6. U.S. Environmental Protection Agency, Office of Research and Development. Scientific and Technical Assessment Report on Particulate Polycyclic Organic Matter (POM). Star Series. Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC EPA-600/6-74-001 (1975).

CATEGORY 24

HETEROCYCLIC OXYGEN COMPOUNDS

SUBCATEGORY: 24B - Three or More Ring Heterocyclic Oxygen Compounds

Summary of Subcategory

Total number of compounds in subcategory	7
number of parent compounds with subspecies	1
number of subspecies	3
Number of parent compounds with no MEG values	5
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

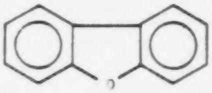
Consent Decree compounds included in subcategory: 0

CATEGORY: 248

DIBENZOFURAN: $C_6H_4OC_6H_4$ (diphenylene oxide). 248020
Colorless crystals.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt:168.21; mp:86-7; bp:287^{760}; d:1.0886^{99}_{4}; vap.d:5.8; slightly soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Dibenzofuran has been reported in samples taken from river water (ref. 1).

Dibenzofuran is an insecticide (ref. 2).

Threshold odor concentration of dibenzofuran in water at room temperature is reported as 0.12 ppm (ref. 3).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for dibenzofuran are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

443<

MULTIMEDIA ENVIRONMENTAL GOALS

24B020
DIBENZOFURAN

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

CATEGORY: 24B

NAPHTHOFURANS: $C_{12}H_8O$ 24B040

NAPHTHO(1,2-b)FURAN:	A solid.	24B041
NAPHTHO(2,1-b)FURAN:	A solid.	24B042
NAPHTHO(2,3-b)FURAN:	A solid.	24B043

PROPERTIES:

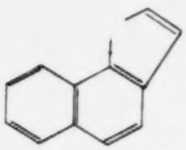
	mol.wt	mp.	bp.
naphtho(1,2-b)furan:	168.19		284
naphtho(2,1-b)furan:	168.19	65	
naphtho(2,3-b)furan:	168.19	120	

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

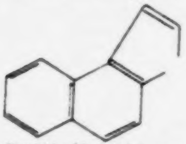
Naphtho(1,2-b)furan and naphtho(2,1-b)furan are present in coal tar (ref. 4).

WLN:

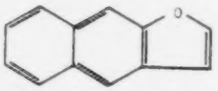
STRUCTURE:



Naphtho(1,2-b)furan



Naphtho(2,1-b)furan



Naphtho(2,3-b)furan

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for naphthofurans are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

24B040
NAPHTHOFURANS

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
Category	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

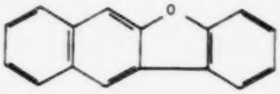
	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

446

CATEGORY: 248
BENZO(b)NAPHTHO(2,3-d)FURAN; $C_{16}H_{10}O$
(β-brazan). 248060
A solid.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 218.26; mp: 209.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzo(b)naphtho(2,3-d)furan is present in coal tar and is a degradation product of brazilin. On oxidation it yields the yellow quinone 2,3-phthaloylbenzofuran (ref. 4).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for benzo(b)naphtho(2,3-d)furan are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

24B060
BENZO(b)NAPHTHO(2,3-d)FURAN

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
Category	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

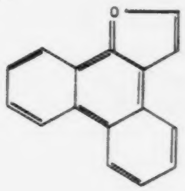
CATEGORY: 248

PHENANTHRO(9,10-b)FURAN: $C_{16}H_{10}O$ 248080

A white solid.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 218.26; mp: 118.5-119.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for phenanthro(9,10-b)furan are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

24B080
PHENANTHRO(9,10-b)FURAN

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
Category	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

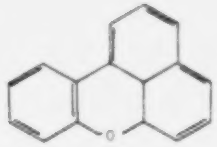
	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

450<

CATEGORY: 24B
1,9-BENZOXANTHENE: $C_{16}H_{10}O$ (benzo-k-xanthene). 24B100
A solid possessing strong blue fluorescence.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 218.26; mp: 109; bp: 395^{758}.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

1,9-Benzoxanthene occurs in coal tar pitch. The compound has been tested as a fungicide and found to demonstrate weak activity (ref. 5).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for 1,9-benzoxanthene are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

24B100

1,9-BENZOXANTHENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
Category	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

REFERENCES: CATEGORY 24B

Heterocyclic Oxygen Compounds - Three or More Ring Heterocyclic Oxygen Compounds

1. Shackelford, W. M., and L. H. Keith. Frequency of Organic Compounds Identified in Water. EPA Publication No. 600/4-76-062, December 1976.

2. Sax, N. I., Ed. Dangerous Properties of Industrial Materials, Fourth Edition. Van Nostrand Reinhold Co., New York, NY (1975).

3. Verschueren, K. Handbook of Environmental Data on Organic Chemicals. Van Nostrand Rheinhold Company, NY (1977).

4. Livingstone, R. Compounds Containing a Five-Membered Ring with One Hetero Atom of Group VI: Oxygen. *Rodd's Chemistry of Carbon Compounds, Second Edition, Vol. 4, Part A*, S. Coffey, Ed., Elsevier Scientific Publishing Company, Amsterdam (1973).

5. Coles, G. Annual Reports of the Agricultural Research Station, Bristol, 101-102 (1956).

CATEGORY 25

HETEROCYCLIC S COMPOUNDS

SUBCATEGORY: 25A - One Ring Heterocyclic S Compounds

Summary of Subcategory

Total number of compounds in subcategory	8
number of parent compounds with subspecies	3
number of subspecies	5
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

Consent Decree compounds included in subcategory: 0

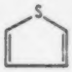
CATEGORY: 25A

WLN: T5SJ

THIOPHENE: C_4H_4S (thiofuran). 25A020

Clear, colorless liquid; disagreeable odor.

STRUCTURE:



PROPERTIES:

Molecular wt: 84.14; mp: 29.8; bp: 84; d: 1.06494;
vap. press: 40 mm at 12.5°; vap. d: 2.9.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Thiophene occurs in small amounts in coal tar. Pyrolysis of thiophene at 800° to 825° gives methane, hydrogen sulfide, and hydrogen as the only gaseous products. In the presence of orthophosphoric acid, thiophene polymerizes to give oligomers (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

No information is available on the possible toxic effects of thiophene.

LC_{Lo} (inhalation, mouse): 8,700 ppm (ref. 2).

LD_{Lo} (intraperitoneal, mouse): 100 mg/kg (ref. 2).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 100 = 4.5 \times 10^3$ μg/m^3
Water, Health: $15 \times 4.5 \times 10^3 = 6.75 \times 10^4$ μg/ℓ
Land, Health: $0.2 \times 6.75 \times 10^5 = 1.35 \times 10^5$ μg/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 100 = 11$ μg/m^3
$EPC_{AH3} = 0.081 \times 100 = 8$ μg/m^3
$EPC_{WH1} = 15 \times 8 = 120$ μg/ℓ
$EPC_{WH2} = 0.4 \times 100 = 40$ μg/ℓ
$EPC_{LH} = 0.2 \times 40 = 8.0$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

25A020
THIOPHENE

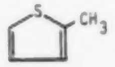
EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			4.5E3		8		
Water, $\mu g/l$ (ppm Wt)			6.75E4		40		
Land, $\mu g/g$ (ppm Wt)			1.35E5		8		

*To be multiplied by dilution factor

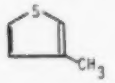
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			8		
Water, $\mu g/l$ (ppm Wt)			40		
Land, $\mu g/g$ (ppm Wt)			8		

WLN: T5SJ B, T5SJ C

STRUCTURE:



2-Methylthiophene



3-Methylthiophene

CATEGORY: 25A

METHYLTHIOPHENES: 25A040

2-METHYLTHIOPHENE, C_5H_6S. 25A041

3-METHYLTHIOPHENE, C_5H_6S. 25A042

Colorless liquids, disagreeable odor.

PROPERTIES:

Molecular wt: 98.17; bp: 112, 114^{738} mm.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

2-Methylthiophene and 3-methylthiophene are found in coal tar. Methylthiophene polymerizes at high temperatures to form oligomers. Oxidation of alkyl thiophenes gives thiophenecarboxylic acids in low yield (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

No information is available on the possible toxic effects of methylthiophenes.

LD_{50} (intraperitoneal, mouse): 500 mg/kg for 2-methylthiophene (ref. 2).

LD_{50} (intraperitoneal, mouse): 512 mg/kg for 3-methylthiophene (ref. 2).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 500 = 2.25 \times 10^4$ µg/m^3

Water, Health: $15 \times 2.25 \times 10^4 = 3.4 \times 10^5$ µg/ℓ

Land, Health: $0.2 \times 3.4 \times 10^5 = 7.0 \times 10^4$ µg/g

Air, Ecology:

Water, Ecology:

Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 500 = 54$ µg/m^3

$EPC_{AH3} = 0.081 \times 500 = 41$ µg/m^3

$EPC_{WH1} = 15 \times 41 = 615$ µg/ℓ

$EPC_{WH2} = 0.4 \times 500 = 200$ µg/ℓ

$EPC_{LH} = 0.2 \times 200 = 40$ µg/g

457<

MULTIMEDIA ENVIRONMENTAL GOALS

25A040
METHYLTHIOPHENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.25E4		41		
Water, $\mu g/l$ (ppm Wt)			3.4E5		200		
Land, $\mu g/g$ (ppm Wt)			7.0E4		40		

*To be multiplied by dilution factor

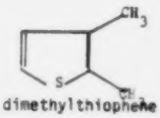
AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			41		
Water, $\mu g/l$ (ppm Wt)			200		
Land, $\mu g/g$ (ppm Wt)			40		

CATEGORY: 25 A

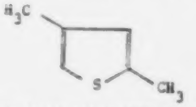
WLN:

DIMETHYLTHIOPHENES: $(CH_3)_2C_4H_2S$ 25A060
2,3-DIMETHYLTHIOPHENE: (2,3-thioxene). A liquid. 25A061
2,4-DIMETHYLTHIOPHENE: (2,4-thioxene). A liquid. 25A062
2,5-DIMETHYLTHIOPHENE: (α,α-thioxene). A liquid. 25A063
3,4-DIMETHYLTHIOPHENE: (3,4-diMe-thiophene). A liquid. 25A064

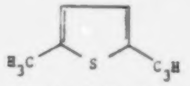
STRUCTURE:



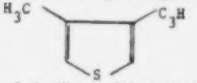
2,3 dimethylthiophene



2,4 dimethylthiophene



2,5 dimethylthiophene



3,4 dimethylthiophene

PROPERTIES:

	mol. wt.	mp.	bp.	d.	solubility in water
2,3-dimethylthiophene:	112.21	-49	141.6^{760}	1.0021_{4}^{20}	insoluble
2,4-dimethylthiophene:	112.21		140.7^{760}	0.9956_{4}^{28}	insoluble
2,5-dimethylthiophene:	112.21	-62.6	136.7^{760}	0.9853_{4}^{20}	insoluble
3,4-dimethylthiophene:	112.21		144-6	1.0084[illegible]	

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

TOXIC PROPERTIES, HEALTH EFFECTS:

When 2,4-dimethylthiophene is heated to decomposition, toxic sulfur fumes are released (ref. 1).

Toxicological data for dimethylthiophenes are not available at this time. However, toxicological characteristics are likely to be similar to those of methylthiophene because of the similarity with regard to structure, and because methylation of thiophene does not appear to increase its toxicity.

LD_{50} (intraperitoneal, mouse): 500 mg/kg for 2-methylthiophene (ref. 2).
LD_{50} (intraperitoneal, mouse): 512 mg/kg for 3-methylthiophene (ref. 2).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

***MINIMUM ACUTE TOXICITY CONCENTRATIONS**:

Air, Health: $45 \times 573 = 2.58 \times 10^4$ μg/m^3 — Air, Ecology:
Water, Health: $15 \times 2.58 \times 10^4 = 3.87 \times 10^5$ μg/l — Water, Ecology:
Land, Health: $0.2 \times 3.87 \times 10^5 = 7.74 \times 10^4$ μg/g — Land, Ecology:

***ESTIMATED PERMISSIBLE CONCENTRATIONS**:

$EPC_{AH2} = 0.107 \times 573 = 61.31$ μg/m^3
$EPC_{AH3} = 0.081 \times 573 = 46.41$ μg/m^3
$EPC_{WH1} = 15 \times 46.41 = 696.2$ μg/l
$EPC_{WH2} = 0.4 \times 573 = 229.2$ μg/l
$EPC_{LH} = 0.2 \times 229.2 = 46$ μg/g

*Based on the LD_{50} (intraperitoneal, mouse): 500 mg/kg for 2-methythiophene;
molecular wt. ratio = $\frac{112.21 \text{ (dimethylthiophenes)}}{98 \text{ (methylthiophene)}} = 1.145$

MULTIMEDIA ENVIRONMENTAL GOALS

25A060
DIMETHYLTHIOPHENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.6E4		46		
Water, $\mu g/l$ (ppm Wt)			3.9E5		229		
Land, $\mu g/g$ (ppm Wt)			7.7E4		46		

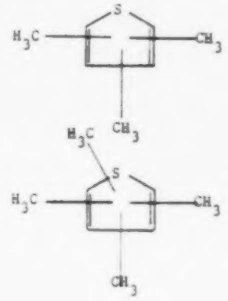
*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			46		
Water, $\mu g/l$ (ppm Wt)			229		
Land, $\mu g/g$ (ppm Wt)			46		

CATEGORY: 25A
TRIMETHYL AND TETRAMETHYL THIOPHENES: 25A080
2,3,5-TRIMETHYLTHIOPHENE: $C_7H_{10}S$. A liquid. 25A081

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 126.22; bp: 164.5^{760}; d: 0.9753^{20}_{4}; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for trimethyl and tetramethyl thiophenes are not available at this time. However, toxicological characteristics are likely to be similar to those of methylthiophene because of the similarity with regard to structure, and because methylation of thiophene does not appear to increase its toxicity.

LD_{50} (intraperitoneal, mouse): 500 mg/kg for 2-methylthiophene (ref. 2).
LD_{50} (intraperitoneal, mouse): 512 mg/kg for 3-methylthiophene (ref. 2).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

*MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health:	$45 \times 644 = 2.90 \times 10^4$ μg/m^3	Air, Ecology:	
Water, Health:	$15 \times 2.90 \times 10^4 = 4.35 \times 10^5$ μg/l	Water, Ecology:	
Land, Health:	$0.2 \times 4.35 \times 10^5 = 8.7 \times 10^4$ μg/g	Land, Ecology:	

*ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 644 = 68.9$ μg/m^3

$EPC_{AH3} = 0.081 \times 644 = 52.2$ μg/m^3

$EPC_{WH1} = 15 \times 52.2 = 783$ μg/l

$EPC_{WH2} = 0.4 \times 644 = 257.6$ μg/l

$EPC_{LH} = 0.2 \times 257.6 = 51.5$ μg/g

*Based on the LD_{50} (intraperitoneal, mouse): 500 mg/kg for 2-methylthiophene;

molecular weight ratio = $\frac{126.22 \text{ (trimethylthiophenes}}{98 \text{ (methylthiophene)}}$ = 1.288

MULTIMEDIA
ENVIRONMENTAL
GOALS

25A080
TRIMETHYL & TETRAMETHYL THIOPHENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent †		B. Ambient Level Goal* †		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.9E4		52		
Water, $\mu g/l$ (ppm Wt)			3.4E5		258		
Land, $\mu g/g$ (ppm Wt)			8.7E4		252		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration †		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			52		
Water, $\mu g/l$ (ppm Wt)			258		
Land, $\mu g/g$ (ppm Wt)			52		

†Based on data for 2-methylthiophene.

REFERENCES: CATEGORY 25A

Heterocyclic S Compounds - One Ring Heterocyclic S Compounds

1. Livingstone, R. Compounds with Five-Membered Rings Having One Hetero Atom from Group VI: Sulphur and Its Analogues. *Rodd's Chemistry of Carbon Compounds, Second Edition, Vol. 4, Part A*, S. Coffey, Ed., Elsevier Scientific Publishing Company, Amsterdam (1973).

2. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

CATEGORY 25

HETEROCYCLIC S COMPOUNDS

SUBCATEGORY: 25B - Two or More Ring Heterocyclic S Compounds

Summary of Subcategory

Total number of compounds in subcategory	6
number of parent compounds with subspecies	1
number of subspecies	3
Number of parent compounds with no MEG values	3
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

Consent Decree compounds included in subcategory: 0

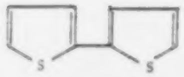
CATEGORY: 25B

2,2'-BITHIOPHENE: $C_8H_6S_2$ (2,2'-bithienyl). 25B020

A solid or liquid.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 166.27; mp: 33; bp: 260^{760}; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

2,2'-Bithiophene has been isolated from togetes roots (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

2,2'-Bithiophene is reported to be an active nematocide, fungicide, and weed killer (ref. 1). The median lethal dose (M.L.D.) for *Heterodura rostochiensis* is reported as 100 ppm (ref. 1).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

25B020
2,2′-BITHIOPHENE

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
Category	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

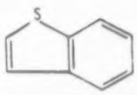
CATEGORY: 25B

BENZO(b)THIOPHENE: C_8H_6S (benzothiofuran, 2,3-benzothiophene, thionaphthene). 25B040

Colorless liquid; naphthalene-like odor.

WLN: T56 BSJ

STRUCTURE:



PROPERTIES:

Molecular wt: 134.20; mp: 32; bp: 221-2; volatile in steam; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Benzo(b)thiophene is present in lignite tar.

TOXIC PROPERTIES, HEALTH EFFECTS:

No information is available on the possible toxic effects of benzo(b)thiophene.

LD_{Lo} (intraperitoneal, mouse): 512 mg/kg (ref. 4).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 512 = 2.3 \times 10^4$ μg/m^3
Water, Health: $15 \times 2.3 \times 10^4 = 3.5 \times 10^5$ μg/ℓ
Land, Health: $0.2 \times 3.5 \times 10^5 = 7.0 \times 10^4$ μg/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 512 = 55$ μg/m^3
$EPC_{AH3} = 0.081 \times 512 = 41$ μg/m^3
$EPC_{WH1} = 15 \times 41 = 615$ μg/ℓ
$EPC_{WH2} = 0.4 \times 512 = 205$ μg/ℓ
$EPC_{LH} = 0.2 \times 205 = 40$ μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

25B040
BENZO(b)THIOPHENE

EMISSION LEVEL GOALS

	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			2.3E4		41		
Water, $\mu g/l$ (ppm Wt)			3.5E5		205		
Land, $\mu g/g$ (ppm Wt)			7.0E4		40		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS

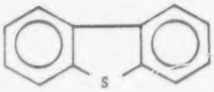
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			41		
Water, $\mu g/l$ (ppm Wt)			205		
Land, $\mu g/g$ (ppm Wt)			40		

CATEGORY: 25B

DIBENZOTHIOPHENE: $C_{12}H_8S$. 25B060
(diphenylene sulfide).
A solid.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt: 184.27; mp: 99-100; bp: 332-3;
Soluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Dibenzothiophene has been reported in samples taken from river water (ref. 2).

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for dibenzothiophene are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

MULTIMEDIA ENVIRONMENTAL GOALS

25B060
DIBENZOTHIOPHENE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

CATEGORY: 25B

BENZONAPHTHATHIOPHENES: $C_{16}H_{10}S$ 25B080

BENZO(b)NAPHTHO(2,3-d)THIOPHENE: 25B081
BENZO(b)NAPHTHO(1,2-d)THIOPHENE: A solid. 25B082
BENZO(b)NAPHTHO(2,1-d)THIOPHENE: A solid. 25B083

PROPERTIES:

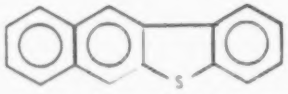
	mol.wt.	mp.
benzo(b)naphtho(2,3-d)thiophene:	234.32	160
benzo(b)naphtho(1,2-d)thiophene:	234.32	185-6
benzo(b)naphtho(2,1-d)thiophene:	234.32	185-6

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

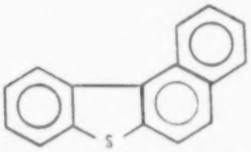
Benzonaphthathiophenes are found to occur in coal tar (ref. 3).

WLN:

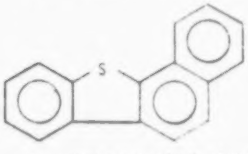
STRUCTURE:



Benzo(b)naptho(2,3-d)thiophene



Benzo(b)naphtho(1,2-d)thiophene



Benzo(b)naphtho(2,1-d)thiophene

TOXIC PROPERTIES, HEALTH EFFECTS:

Toxicological data for benzonaphthothiophenes are not available at this time.

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

471<

MULTIMEDIA ENVIRONMENTAL GOALS

25B080
BENZONAPHTHOTHIOPHENES

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)							
Water, $\mu g/l$ (ppm Wt)							
Land, $\mu g/g$ (ppm Wt)							

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)					
Water, $\mu g/l$ (ppm Wt)					
Land, $\mu g/g$ (ppm Wt)					

REFERENCES: CATEGORY 25B

Heterocyclic S Compounds -
Two or More Ring Heterocyclic S Compounds

1. Whlenbrock, J. Rendeous Transaction Chimie, 78: 382-390 (1954).

2. Shackelford, W. M., and L. H. Keith. Frequency of Organic Compounds Identified in Water. Environmental Protection Agency, EPA-600/4-76-062, Dec. 1976.

3. Kruber, R. Chemische Berichte, Vol. 73, p. 1184 (1940).

4. Christensen, H. E., and E. J. Fairchild. Registry of Toxic Effects of Chemical Substances: 1976 Edition. Prepared by Tracor Jitco Inc., Rockville, MD for National Institute for Occupational Safety and Health. HEW Publication No. (NIOSH) 76-191 (1976).

CATEGORY 26

ORGANOPHOSPHOROUS COMPOUNDS

SUBCATEGORY: 26A - Aliphatic Organophosphorous Compounds

Summary of Subcategory

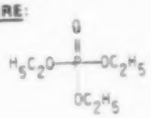
Total number of compounds in subcategory	1
number of parent compounds with subspecies	0
number of subspecies	0
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

Consent Decree compounds included in subcategory: 0

CATEGORY: 26A

WLN: $2OPO\&O_2\&O_2$

STRUCTURE:



TRIETHYL PHOSPHATE: $C_6H_{15}O_4P$. 26A020.
(Ethyl phosphate)
Liquid.

PROPERTIES:

Molecular wt.: 182.16; bp: 215-216; mp: -56.5°C; d: $1.067\text{-}1.072^{20}_{20}$; vap. d: 6.28; vap. press: 1 mm at 39.6°C; insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Used as an ethylating agent in the formation of polyesters which are used in insecticides (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

Triethyl phosphate causes choline esterase inhibition and may be expected to cause nerve injury similar to that of other phosphate esters (ref. 2). It is an anesthetic, producing muscle relaxation in high dosages (ref. 3). Slight irritant properties to guinea pigs are reported (ref. 3).

LD_{53} (Oral, rat): >0.8 g/kg (ref. 3).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $45 \times 800 = 3.6 \times 10^4$ μg/m³
Water, Health: $14 \times 3.6 \times 10^4 = 5.4 \times 10^5$ μg/l
Land, Health: $0.2 \times 5.4 \times 10^5 = 1.08 \times 10^5$ μg/g

Air, Ecology:
Water, Ecology:
Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

$EPC_{AH2} = 0.107 \times 800 = 84.6$ μg/m³
$EPC_{AH3} = 0.081 \times 800 = 64.8$ μg/m³
$EPC_{WH1} = 15 \times 64.8 = 972$ μg/l
$EPC_{WH2} = 0.4 \times 800 = 320$ μg/l
$EPC_{LH} = 0.2 \times 320 = 64$ μg/g

475<

MULTIMEDIA ENVIRONMENTAL GOALS

26A020
TRIETHYL PHOSPHATE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			3.6E4		64.8		
Water, $\mu g/l$ (ppm Wt)			5.4E5		320		
Land, $\mu g/g$ (ppm Wt)			1.08E5		64		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			64.8		
Water, $\mu g/l$ (ppm Wt)			320		
Land, $\mu g/g$ (ppm Wt)			64		

REFERENCES: CATEGORY 26A

Organophosphorous Compounds - Aliphatic Organophosphorous Compounds

1. Windholz, M., Ed. The Merck Index: An Encyclopedia of Chemicals and Drugs, Ninth Edition. Merck & Co., Inc., Rahway, NJ (1976).

2. Sax, N. I., Ed. Dangerous Properties of Industrial Materials, Fourth Edition. Van Nostrand Reinhold Co., New York, NY (1975).

3. Fasset, D. W. Esters, *Industrial Hygiene and Toxicology, Second Revised Edition, Vol. 2*, F. A. Patty, Ed., Interscience Publishers, New York, *p. 1847-1933* (1962).

CATEGORY 26

ORGANOPHOSPHOROUS COMPOUNDS

SUBCATEGORY: 26B - Aromatic Organophosphorous Compounds

Summary of Subcategory

Total number of compounds in subcategory	4
number of parent compounds with subspecies	1
number of subspecies	3
Number of parent compounds with no MEG values	0
Number of parent compounds with natural background levels only	0
Number of parent compounds with Ambient Level Goals based on evidence of carcinogenicity or teratogenicity	0

Consent Decree compounds included in subcategory: 0

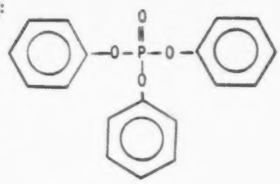
CATEGORY: 26B

TRIPHENYL PHOSPHATE: $C_{18}H_{15}O_4P$. 26B020

Colorless, odorless, crystalline solid.

WLN:

STRUCTURE:



PROPERTIES:

Molecular wt.: 326.28; bp: 245°; mp: 48.5°; d: 1.268; vp: <0.1 mm at 30°C.

Insoluble in water.

NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Noncombustible substitute for camphor in celluloid. The compound is also used as a plasticizer in lacquer and varnishes (ref. 1), a gasoline additive, flotation agent, antioxidant and surfactant (ref. 2).

TOXIC PROPERTIES, HEALTH EFFECTS:

Triphenyl phosphate is slowly absorbed, and acute toxicity is low (refs. 3,4). There was no evidence of adverse clinical effects in men exposed for as long as ten years to triphenyl phosphate vapor, mist, and dust at a weighted average concentration of 3.5 mg/m^3 (ref. 3).

LD_{Lo}: 3,000 mg/m^3 (ref. 5).

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV 3 mg/m^3

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $10^3 \times 3 = 3.0 \times 10^3$ µg/m^3

Water, Health: $15 \times 3.0 \times 10^3 = 4.5 \times 10^4$ µg/l

Land, Health: $0.2 \times 4.5 \times 10^4 = 9.0 \times 10^3$ µg/g

Air, Ecology:

Water, Ecology:

Land, Ecology:

ESTIMATED PERMISSIBLE CONCENTRATIONS:

EPC_{AH1} = $10^3 \times 3/420 = 7.14$ µg/m^3

EPC_{WH1} = $15 \times 7.14 = 107.14$ µg/l

EPC_{WH2} = $13.8 \times 3 = 41.4$ µg/l

EPC_{LH} = $0.2 \times 41.4 = 8.3$ µg/g

MULTIMEDIA ENVIRONMENTAL GOALS

26B020

TRIPHENYL PHOSPHATE

EMISSION LEVEL GOALS							
	I. Based on Best Technology		II. Based on Ambient Factors				
	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, $\mu g/m^3$ (ppm Vol)			3.0E3		7.14		
Water, $\mu g/l$ (ppm Wt)			4.5E4		41.4		
Land, $\mu g/g$ (ppm Wt)			9.0E3		8.3		

*To be multiplied by dilution factor

AMBIENT LEVEL GOALS					
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, $\mu g/m^3$ (ppm Vol)			7.14		
Water, $\mu g/l$ (ppm Wt)			41.4		
Land, $\mu g/g$ (ppm Wt)			8.3		

CATEGORY: 26B

TRITOLYL PHOSPHATE: $C_{21}H_{21}O_4P$. (tri-cresol phosphate) 26B040
TRI-o-TOLYL PHOSPHATE: (tri-o-cresyl-phosphate, triorthocresol phosphate) 26B041
TRI-m-TOLYL PHOSPHATE: 26B042
TRI-p-TOLYL PHOSPHATE: 26B043

Oily, flame-resistant liquid.

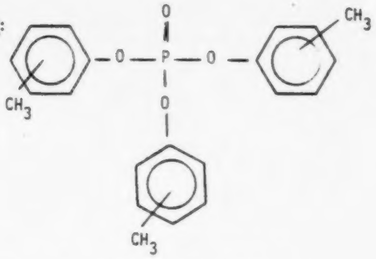
PROPERTIES:

Molecular wt.: 368.36; bp: 265°.

Insoluble in water.

WLN:

STRUCTURE:



NATURAL OCCURRENCE, CHARACTERISTICS, ASSOCIATED COMPOUNDS:

Used as a plasticizer in vinyl plastic manufacture, as a flame-retardant, as a solvent for nitro cellulose, and as an additive in gasoline and extreme pressure lubricants (ref. 1).

TOXIC PROPERTIES, HEALTH EFFECTS:

The ortho isomer is highly toxic (ref. 3). It probably inhibits pseudocholine esterase and thereby affects the central nervous system to cause paralysis (refs. 4,6). The lowest lethal dose for the ortho isomer has been reported to be 1,000 mg/kg for humans when ingested orally (ref. 5).

Tritolyl phosphate: LD_{Lo} (oral, rat): 4,680 mg/kg (ref. 5).
Tri-o-tolyl phosphate: LD_{50} (oral, rat): 3 g/kg (ref. 4).
Tri-p-tolyl phosphate: LD_{50} (oral, rat): 12.8 g/kg (ref. 4).
Aquatic toxicity (tritolyl phosphate): TLm_{96}: 10-1 ppm (ref. 5)

REGULATORY ACTIONS, STANDARDS, CRITERIA, RECOGNITION, CANDIDATE STATUS FOR SPECIFIC REGULATION:

TLV: 0.1 mg/m^3 for the ortho-isomer.

MINIMUM ACUTE TOXICITY CONCENTRATIONS:

Air, Health: $10^3 \times 0.1 = 1.0 \times 10^2$ μg/m^3
Water, Health: $15 \times 1.0 \times 10^2 = 1.5 \times 10^3$ μg/ℓ
Land, Health: $0.2 \times 1.5 \times 10^3 = 3.0 \times 10^2$ μg/g

Air, Ecology:
Water, Ecology: 100 x 1 = 100 μg/1
Land, Ecology: 0.2 x 100 = 20 μg/g

ESTIMATED PERMISSIBLE CONCENTRATIONS:

EPC_{AH1} = $10^3 \times 0.1/420 = 0.24$ μg/m^3
EPC_{WH1} = 15 x 0.24 = 3.57 μg/ℓ
EPC_{WH2} = 13.8 x 0.1 = 1.38 μg/ℓ
EPC_{LH} = 0.2 x 1.38 = 0.28 μg/g

EPC_{WE1} = 50 x 1 = 50 μg/1
EPC_{LE} = 0.2 x 50 = 10 μg/g

MULTIMEDIA ENVIRONMENTAL GOALS

X
26B040
TRITOLYL PHOSPHATE

	EMISSION LEVEL GOALS						
	I. Based on Best Technology		II. Based on Ambient Factors				
Category	A. Existing Standards	B. Developing Technology	A. Minimum Acute Toxicity Effluent		B. Ambient Level Goal*		C. Elimination of Discharge
	NSPS, BPT, BAT	Engineering Estimates (R&D Goals)	Based on Health Effects	Based on Ecological Effects	Based on Health Effects	Based on Ecological Effects	Natural Background*
Air, μg/m^3 (ppm Vol)			1.0E2		0.24		
Water, μg/l (ppm Wt)			1.5E3	100	1.38	50	
Land, μg/g (ppm Wt)			3.0E2	20	0.28	10	

*To be multiplied by dilution factor

	AMBIENT LEVEL GOALS				
	I. Current or Proposed Ambient Standards or Criteria		II. Toxicity Based Estimated Permissible Concentration		III. Zero Threshold Pollutants Estimated Permissible Concentration
	A. Based on Health Effects	B. Based on Ecological Effects	A. Based on Health Effects	B. Based on Ecological Effects	Based on Health Effects
Air, μg/m^3 (ppm Vol)			0.24		
Water, μg/l (ppm Wt)			1.38	50	
Land, μg/g (ppm Wt)			0.28	10	

REFERENCES: CATEGORY 26B

Organophosphorous Compounds - Aromatic Organophosphorous compounds

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3. American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values for Substances in Workroom Air with Supplements, Third Edition. American Conference of Governmental Industrial Hygienists, Cincinnati, OH (1974).
4. Fasset, D. W. Esters. Industrial Hygiene and Toxicology, Second Revised Edition, Vol. 2, F. A. Patty, Ed., Interscience Publishers, New York, pp. 1847-1933 (1963).
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